Department of Chemical Engineering

Synthesis of Heat Integrated Resource Conservation Networks

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Declaration

To the best of my knowledge and belief this thesis contains no material previously published by any other person except where due acknowledgment has been made. This thesis contains no material which has been accepted for the award of any other degree or diploma in any university.

Yin Ling Tan
1st July 2013

To my husband and my son with love

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ABSTRACT

Huge amount of energy and fresh resources (i.e. water, chemicals, solvents) are consumed by process industries to achieve the desired product throughput and quality. The current drive toward sustainability and business competitiveness has driven the process industries to effectively use these resources. Thus, resource conservation activities have become the centre of attention as compared to conventional end-of-pipe waste treatment system. Process integration has been commonly used as an effective tool for resource conservation and waste reduction. One of the most established areas of process integration is concentration- and property-based resource conservation networks (RCNs). Most works in RCNs synthesis do not consider temperature as part of process constraints. However, in many cases, temperature is an important design parameter. Thus, simultaneous consideration of mass/property and heat recovery should be addressed. Earlier works in this area have been mainly focusing on heat integrated water networks (HIWNs). However, these methods cannot be applied for property-based RCNs, as they are limited to "chemo-centric" system. Clearly, a more generic approach is needed for the synthesis of concentration- and property-based heat integrated resource conservation networks (HIRCNs). This thesis presents novel and generic methodologies for the synthesis of concentration- and property-based HIRCNs with variable operating parameters (i.e. flowrates, temperatures and properties). Firstly, a new generic overall methodology for concentration- and property-based HIRCNs is established. Next, a general framework for synthesis of HIRCNs with and without heat of mixing is presented. Based on this framework, new methodology for the synthesis of HIRCNs with and without heat of mixing are established respectively. Moreover, a revised floating pinch method is developed for utilities targeting in heat exchanger networks (HENs) with varying temperature range, and it is incorporated in the new methodologies for the synthesis of HIRCNs with and without heat of mixing. Various case studies are solved to illustrate the developed methodologies.

PUBLICATIONS

1. **Tan, Y. L.**, Ng, D. K. S., El-Halwagi, M. M., Foo, D. C. Y and Samyudia, Y. (2013). Synthesis of heat integrated resource conservation networks using variable operating parameters, *Industrial & Engineering Chemistry Research*, 52 (22): 7196-7210.

2. **Tan, Y. L.**, Ng, D. K. S., El-Halwagi, M. M., Foo, D. C. Y and Samyudia, Y., Heat integrated resource conservation networks without mixing prior to heat exchanger network, *Journal of Cleaner Production* (*in review*).

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4. **Tan, Y. L.**, Ng, D. K. S., El-Halwagi, M. M., Foo, D. C. Y and Samyudia, Y., (2013). Heat integrated resource conservation networks without mixing prior to heat exchanger network. 6th International Conference on Process Systems Engineering (PSE Asia 2013), Kuala Lumpur.

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NOMENCLATURE

SETS:

NCOLD	set of cold streams
NCOMP	set of components
NFRESH	set of fresh resources
NHOT	set of hot streams
NPINCH	set of pinch point candidates
NPROP	set of properties
NSINKS	set of process sinks
NSOURCES	set of process sources

INDICES:

c	index for cold streams
h	index for hot streams
i	index for process sources
j	index for process sinks
k	index for components
p	index properties
q	index for pinch point candidates
r	index for fresh resources
waste	index for waste

PARAMETERS:

a_c	parameter in linearised temperature-dependent expression for heat capacity of the pure component; a_c = 1.3724 J/(g K) for water, 0.4685 J/(g K) for phenol
a_{12}	binary parameter in the Wilson equation for phenol and water solution, a_{12} = 2.4395

a_{21}	binary parameter in the Wilson equation for phenol and water solution, a_{21} = -3.2239
b_c	parameter in linearised temperature-dependent expression for heat capacity of the pure component; b_c = 0.0083 J/(g K) for water, 0.0044 J/(g K) for phenol
b_{12}	binary parameter in the Wilson equation for phenol and water solution, b_{12} = -2229.9297 K
b_{21}	binary parameter in the Wilson equation for phenol and water solution; b_{21} = 1046.1246 K
CP_c	heat capacity of a cold stream c
CP_h	heat capacity of a hot stream h
CP_i	heat capacity of process source i
CP_k	heat capacity of component k
CP_r	heat capacity of fresh resource r
Cost_c	unit cost of cold utility
Cost_h	unit cost of hot utility
Cost_r	unit cost of fresh resource r
$\mathrm{Cost}_{\mathrm{waste}}$	unit cost of waste
d_{12}	binary parameter in the NRTL equation for acetone and water solution, d_{12} = 631.05
d_{21}	binary parameter in the NRTL equation for acetone and water solution; d_{21} = 1197.41
$G_j^{\max}$	upper bound total flowrate inlet process sink j
$G_j^{\min}$	lower bound total flowrate inlet process sink j
k	total operating hours per year
$m_c^{\max}$	upper bound flowrate of cold stream c
$m_c^{\min}$	lower bound flowrate of cold stream c
$m_h^{\max}$	upper bound flowrate of hot stream h
$m_h^{\min}$	lower bound flowrate of hot stream h
R	ideal gas constant, is taken as 8.314 J/(Kmol)
$T_{\circ}$	reference temperature, assumed to be 0°C
T_i	temperature of process source i

$T_c^{\text{in, max}}$	upper bound supply temperature of cold stream c
$T_c^{\text{in, min}}$	lower bound supply temperature of cold stream c
$T_c^{\text{out, max}}$	upper bound target temperature of cold stream c
$T_c^{\text{out, min}}$	lower bound target temperature of cold stream c
$T_h^{\text{in, max}}$	upper bound supply temperature of hot stream h
$T_h^{\text{in, min}}$	lower bound supply temperature of hot stream h
$T_h^{\text{out, max}}$	upper bound target temperature of hot stream h
$T_h^{\text{out, min}}$	lower bound target temperature of hot stream h
$T_j^{\max}$	upper bound temperature of process sink j
$T_j^{\min}$	lower bound temperature of process sink j
T_r	temperature of fresh resource r
U_c	maximum flowrate of cold stream c
U_h	maximum flowrate of hot stream h
W_i	total flowrate from process source i
$\Delta T_{\min}$	minimum temperature difference
α	parameter in NRTL equation for acetone and water, $\alpha = 0.5343$
$\psi_{i,p}$	property operator p of process source i
$\psi_{j,p}^{\max}$	upper bound property operator p of process sink j
$\psi_{j,p}^{\min}$	lower bound property operator p of process sink j
$\psi_{r,p}$	property operator p of fresh resource r

VARIABLES:

B_{waste}	flowrate of waste
$B_{c,\text{waste}}$	flowrate of cold stream c to waste
$B_{h,\text{waste}}$	flowrate of hot stream h to waste
$B_{i,\text{waste}}$	flowrate of process source i to waste
$CP_{i,j}^{\text{C}}$	heat capacity of cold stream c from source i to sink j

$CP^{\mathrm{C}}_{i,\mathrm{waste}}$	heat capacity of cold stream c from source i to waste
$CP^{\mathrm{C}}_{r,j}$	heat capacity of cold stream c from fresh resource r to sink j
$CP^{\mathrm{H}}_{i,j}$	heat capacity of hot stream h from source i to sink j
$CP^{\mathrm{H}}_{i,\mathrm{waste}}$	heat capacity of hot stream h from source i to waste
$CP^{\mathrm{H}}_{r,j}$	heat capacity of hot stream h from fresh resource r to sink j
CP_j	heat capacity of process sink j
CP_k	heat capacity of component k
CP_{waste}	heat capacity of waste
F_r	flowrate of fresh resource r
$f_{r,c}$	flowrate of fresh resource r to cold stream c
$f_{r,h}$	flowrate of fresh resource r to hot stream h
$f_{r,j}$	flowrate of fresh resource r to process sink j
G_j	total flowrate inlet process sink j
$g_{c,j}$	flowrate of cold stream c to process sink j
$g_{h,j}$	flowrate of hot stream h to process sink j
m_c	flowrate of cold stream c
m_h	flowrate of hot stream h
$m^{\mathrm{C}}_{i,j}$	flowrate of cold stream c from source i to sink j
$m^{\mathrm{C}}_{i,\mathrm{waste}}$	flowrate of cold stream c from source i to waste
$m^{\mathrm{C}}_{r,j}$	flowrate of cold stream c from fresh resource r to sink j
$m^{\mathrm{H}}_{i,j}$	flowrate of hot stream h from source i to sink j
$m^{\mathrm{H}}_{i,\mathrm{waste}}$	flowrate of hot stream h from source i to waste
$m^{\mathrm{H}}_{r,j}$	flowrate of hot stream h from fresh resource r to sink j
Q_c	external cold utility
Q_h	external hot utility
T^{in}_c	supply temperature of cold stream c
T^{out}_c	target temperature of cold stream c
T^{s}_c	shifted supply temperature of cold stream c
T^{t}_c	shifted target temperature of cold stream c

$T_{r,j}^{\mathrm{C,in}}$	supply temperatures of cold stream *c* from fresh resource *r* to sink *j*
$T_{i,j}^{\mathrm{C,in}}$	supply temperatures of cold stream *c* from source *i* to sink *j*
$T_{i,\mathrm{waste}}^{\mathrm{C,in}}$	supply temperatures of cold stream *c* from source *i* to waste
$T_{r,j}^{\mathrm{C,out}}$	target temperatures of cold stream *c* from fresh resource *r* to sink *j*
$T_{i,j}^{\mathrm{C,out}}$	target temperatures of cold stream *c* from source *i* to sink *j*
$T_{i,\mathrm{waste}}^{\mathrm{C,out}}$	target temperatures of cold stream *c* from source *i* to waste
T_{h}^{in}	supply temperature of hot stream *h*
T_{h}^{out}	target temperature of hot stream *h*
T_{h}^{s}	shifted supply temperature of hot stream *h*
T_{h}^{t}	shifted target temperature of hot stream *h*
$T_{r,j}^{\mathrm{H,in}}$	supply temperatures of hot stream *h* from fresh resource *r* to sink *j*
$T_{i,j}^{\mathrm{H,in}}$	supply temperatures of hot stream *h* from source *i* to sink *j*
$T_{i,\mathrm{waste}}^{\mathrm{H,in}}$	supply temperatures of hot stream *h* from source *i* to waste
$T_{r,j}^{\mathrm{H,out}}$	target temperatures of hot stream *h* from fresh resource *r* to sink *j*
$T_{i,j}^{\mathrm{H,out}}$	target temperatures of hot stream *h* from source *i* to sink *j*
$T_{i,\mathrm{waste}}^{\mathrm{H,out}}$	target temperatures of hot stream *h* from source *i* to waste
T_{j}	temperature of process sink *j*
T_{q}	potential pinch point candidate *q*
T^{waste}	temperature of waste
Tox	toxicity
THOD	theoretical oxygen demand
$w_{i,c}$	flowrate of process source *i* to cold stream *c*
$w_{i,h}$	flowrate of process source *i* to hot stream *h*
$w_{i,j}$	flowrate of process source *i* to process sink *j*
x_k	mole fraction of component *k*
x_m	mole fraction of stream *m*
$\psi(\overline{p})$	property operator *p* of mixture property $\overline{p}$

$\psi_{c,p}$	property operator p of cold stream c
$\psi_{h,p}$	property operator p of hot stream h
$\psi_{j,p}$	property operator p of process sink j
$\psi_{m,p}$	property operator p of stream m
$\psi_{\mathrm{HEN},p}^{\min}$	minimum property operator p in HEN
$\psi_{\mathrm{HEN},p}^{\max}$	maximum property operator p in HEN
$\psi_{\mathrm{waste},p}$	maximum property operator p of waste
ρ	density
μ	viscosity
$\Delta H_{c}^{\mathrm{mix}}$	heat of mixing of cold stream c
$\Delta H_{h}^{\mathrm{mix}}$	heat of mixing of hot stream h
$\Delta H_{j}^{\mathrm{mix}}$	heat of mixing of sink j
Λ_{12}, Λ_{21}	binary variables in the Wilson equation
ϕ_c	binary variable for cold stream c
ϕ_h	binary variable for hot stream h
$\beta_{h,q}^{\mathrm{t}}$, $\beta_{h,q}^{\mathrm{s}}$	binary variables in the energy balance equation above the pinch point candidates
$\gamma_{c,q}^{\mathrm{t}}$, $\gamma_{c,q}^{\mathrm{s}}$	binary variables in the energy balance equation above the pinch point candidates
$\lambda_{h,q}^{\mathrm{t}}$, $\lambda_{h,q}^{\mathrm{s}}$	binary variables in the energy balance equation below the pinch point candidates
$\eta_{c,q}^{\mathrm{t}}$, $\eta_{c,q}^{\mathrm{s}}$	binary variables in the energy balance equation below the pinch point candidates

CHAPTER 1: INTRODUCTION

1.1 Background and motivation

Traditionally, process industries have been focusing on conventional end-of-pipe waste treatment. Over the past decades, the centre of attention has shifted towards sustainable operations with resource conservation activities. Amongst the few reasons that have resulted in this change include environmental sustainability, stringent emission legislation as well as the increase of fresh resources and waste treatment costs.

Process integration has been commonly used as an effective tool for resource conservation and waste reduction. El-Halwagi (2006) defines process integration as *a holistic approach to process design, retrofitting and operation which emphasises the unity of the process*. Process integration can be generally categorised as heat and mass integrations. Heat integration is *a systematic methodology that provides a global understanding of heat utilisation within the process and employs this understanding in identifying the utility targets and optimising heat recovery as well as energy-utility systems* (El-Halwagi, 2006). Extensive reviews on energy can be found in Linnhoff et al. (1982), Gundersen and Naess (1988), Linnhoff (1993), Furman and Sahinidis (2002), Smith (2005), Kemp (2007) and Klemeš et al. (2010).

On the other hand, mass integration is *a systematic approach that provides a fundamental understanding of the global flow of mass within the process and employs the understanding in identifying performance targets and optimising the generation and routine of species throughout the process* (El-Halwagi, 2006). One of the most established area for mass integration is resource conservation networks (RCNs). Extensive works have been reported in the area of water network synthesis as well as hydrogen network synthesis. Reviews on mass integration were conducted by El-Halwagi and Spriggs (1998), El-Halwagi (2006), El-Halawgi (2012) and Foo (2012).

The significance of mass integration techniques for material reuse and recycle is well established. However, the major drawback of the previous works is that they are limited to "chemo-centric" (Shelley and El-Halwagi, 2000; El-Halwagi, 2006). Note that many design problems are not limited by the nature and quantity of chemical of the streams. Other properties or functionalities of the streams (e.g. pH, density, colour, etc.) are usually involved (El-Halwagi, 2006; Foo, 2012). Furthermore, the effluent regulation is commonly defined not only in term of pollutant concentration but also based on stream properties, such as pH, colour, etc. To overcome this limitation, El-Halwagi and co-workers (Shelley and El-Halwagi, 2000; El-Halwagi et al., 2004) introduced the notion of property integration, which is defined as *a functionality-based, holistic approach to the allocation and manipulation of streams and processing units, which is based on the tracking, adjustment, assignment, and matching functionalities throughout the process*. Various methodologies have also been established for the design of property-based RCNs.

Most works in resource conservation network (RCN) synthesis do not consider temperature as part of process constraints. However, in many cases, temperature is an important design parameter. For example, when solvent is utilised for extraction purpose, heating or cooling is needed to achieve the desired operating conditions before the solvent is fed into the extraction column. Therefore, resource conservation and energy management need to be considered simultaneously as both quality and temperature of solvent are equally important. In addition, in some cases, the property of the solvent may be sensitive to temperature change. Therefore, simultaneous consideration of property and heat recovery should be addressed. Earlier works in this area have been mainly focusing on heat integrated water networks (HIWNs). However, these methods cannot be applied for property-based RCNs, as they are limited to "chemo-centric" system. Clearly, a more generic approach is needed for the synthesis of concentration- and property-based heat integrated resource conservation networks (HIRCNs).

1.2 Objective

The objective of this research is to develop novel and generic methodologies for the synthesis of concentration- and property-based HIRCNs.

1.3 Scopes of research

The scopes of this work include:

i. Floating pinch approach for heat exchanger networks

Development of a revised floating pinch method to identify hot and cold utility targets for heat exchanger networks (HENs) with uncertain and varying temperature and flowrate range will be conducted.

ii. Overall framework for concentration- and property-based HIRCNs synthesis

A new generic overall methodology for concentration- and property-based HIRCNs will be proposed. This methodology provides the overall process on the selection of HIRCNs without and with heat of mixing. In addition, the methodology also evaluates the requirement of heat exchanger network (HEN).

iii. General framework for synthesis of HIRCNs with and without heat of mixing

A general framework for synthesis of HIRCNs with and without heat of mixing will be presented. It serves as a fundamental strategy for the development of methodologies for HIRCNs with and without heat of mixing.

iv. Synthesis of HIRCNs without heat of mixing

A new methodology for the synthesis of HIRCNs without consideration of heat of mixing will be established. In the proposed superstructure, process sources are directly linked to process sinks without prior mixing. The model formulation will be complemented by the revised floating pinch approach to determine the optimum fresh material resources as well as hot and cold utility targets.

v. Synthesis of HIRCNs with heat of mixing

For the synthesis of HIRCNs with heat of mixing, a new methodology will be developed. The proposed superstructure includes all possibilities of stream mixing before HEN, stream splitting after HEN, stream mixing before each sink and sources bypassing the HEN. The optimum fresh material resources as well as hot and cold utility targets will be determined by the model. Note that the model will also integrate the revised floating pinch approach to determine the utility targets.

1.4 Novelty, contribution and significance

This research provides significant contributions in the area of concentration- and property-based HIRCNs synthesis. The main contributions are summarised as follows:

i. As far as it can be found in literature, this is the first work on a more generic approach for HIRCNs that considers both concentration- and property-based systems. The concept of HENs and property-based RCNs constitutes this work. Furthermore, this work can directly be applied to concentration-based HIRCNs as concentration can be considered as a property in a process stream.

ii. This work presents a novel overall methodology for concentration- and property-based HIRCNs synthesis which provides guidance on the selection of the HIRCNs methodologies for with and without heat of mixing based on the type of mixtures in the process streams.

iii. A strategic framework for the development of HIRCNs methodologies for with and without heat of mixing is presented.

iv. A revised mathematical approach based on floating pinch concept for identifying minimum hot and cold utilities is developed for HENs with uncertain or varying range of temperature and flowrate.

v. For the synthesis of HIRCNs without heat of mixing, the methodology is the first work to handle property-based HIRCNs. Furthermore, it is applied to concentration-based HIRCNs as well as HIRCNs with multiple properties.

vi. The methodology for the synthesis of HIRCNs with heat of mixing presented in this thesis is the first work that handles both concentration- and property-based HIRCNs with heat of mixing as well as temperature-interdependence properties. Furthermore, the derived superstructure is a unique and newly presented superstructure found in open literature.

1.5 Summary of the thesis

This thesis is organised as follows.

A review of relevant literatures of this thesis is provided in Chapter 2. The development of various process integration methodologies for the synthesis of HENs, RCNs and HIWNs are critically reviewed.

Chapter 3 describes the overall framework for concentration-based and property-based HIRCNs. The general methodology to synthesise HIRCNs with and without heat of mixing is also addressed.

Methodology for floating pinch for HEN synthesis is presented in Chapter 4. The proposed model is able to identify minimum hot and cold utility targets for heat exchanger networks with varying temperature and flowrate range.

In Chapters 5 and 6, the detailed model formulation for HIRCNs without and with heat of mixing is presented, respectively. Analysis and discussions of results of applying these methodologies on case studies are also included.

Chapter 7 concludes the thesis by summarising the contributions of this work and some recommendations for future developments of HIRCN synthesis. Figure 1.1 summarises the connections between chapters in this thesis.

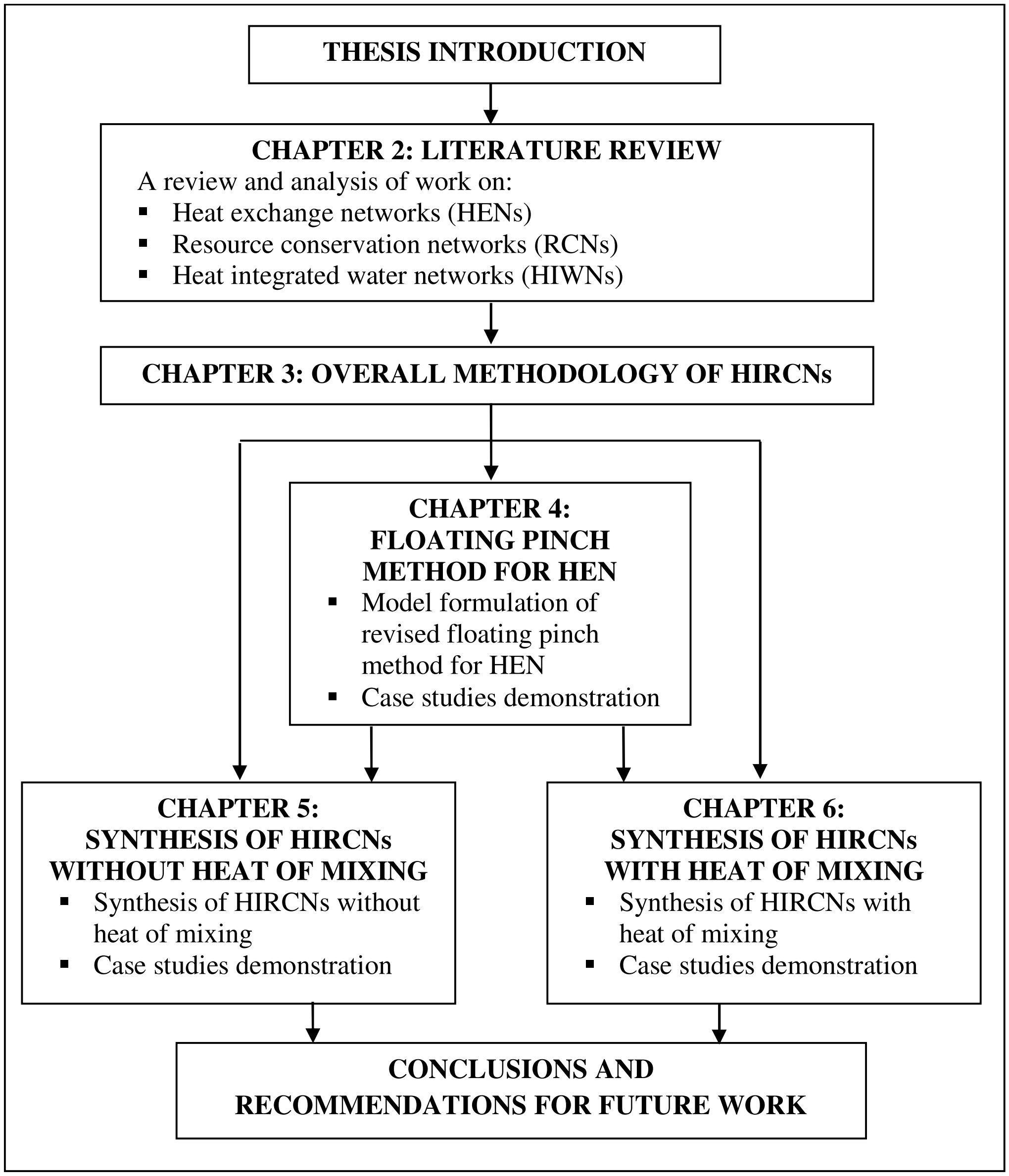


Figure 1.1: A flow diagram illustrating connections among various chapters.

CHAPTER 2: LITERATURE REVIEW

2.1 Introduction

Process integration techniques have been widely accepted as effective tools for resource conservation and waste reduction for the process industry. Available tools of process integration techniques for resource conservation networks (RCNs) can be generally categorised as heat, mass and property integration (El-Halwagi, 2006). Many reviews and textbooks are now available (Gundersen and Naess, 1988; Linnhoff, 1993; El-Halwagi and Spriggs, 1998; Furman and Sahinidis, 2002; Dunn and El-Halwagi, 2003; Foo, 2012). It should be noted that in conventional practise, heat, mass and property integration are carried out independently, i.e. without much interactions among them. Nevertheless, since about a decade ago, extensive works have been reported for the special case of concentration-based heat integrated resource conservation networks (HIRCNs), i.e. heat integrated water networks (HIWNs). However, no work on property-based HIRCNs has been found. The aim of this research is to develop methodologies for HIRCNs. Therefore, it is important to have a firm grasp of heat exchanger networks (HENs), RCNs and HIWNs concepts. This chapter therefore presents a critical review on the state-of-the-art developments in the synthesis of HENs (focusing on minimum utility targeting), RCNs as well as HIWNs.

2.2 Literature review

2.2.1 Heat exchanger networks

Over the past decades, heat exchanger network synthesis has been an important field in process integration. Huge amount of research has been conducted in this area with reviews being reported in Linnhoff et al. (1982), Gundersen and Naess (1988) and Furman and Sahinidis (2002). Most of the contributions in heat exchanger network synthesis can be classified as sequential and simultaneous synthesis methods. The former divides the heat exchanger network synthesis problem into three sub-problems, i.e. minimum utility usage/cost, the minimum number of heat exchanger units, and the minimum area/capital cost of the network, to reduce the computational expensive exercise. Most simultaneous synthesis techniques primarily determine the optimal HEN structure through mixed integer nonlinear programming (MINLP) formulation.

Sequential synthesis approach can further be divided into two subcategories into (i) insight-based *pinch analysis* techniques such as heat transfer composite curves (Hohmann, 1971; Umeda et al., 1978; Umeda et al., 1979), problem table algorithm (Linnhoff and Flower, 1978b; Linnhoff and Flower, 1978a), pinch design method (Linnhoff and Hindmarsh, 1983; Ahmad et al., 1990; Linnhoff and Ahmad, 1990; Linnhoff, 1993), dual temperature (Trivedi et al., 1989a) and pseudo-pinch methods (Rev and Fonyo, 1986b; Rev and Fonyo, 1986a; Trivedi et al., 1989b; Wood et al., 1991) and (ii) mathematical programming techniques (Cerda et al., 1983; Papoulias and Grossmann, 1983; Floudas et al., 1986; Suaysompol and Wood, 1991; Ježowski and Friedler, 1992; Galli and Cerda, 1998a; Galli and Cerda, 1998b; Galli and Cerda, 1998c). The following section mainly focuses on reviewing the minimum utility targeting problem with sequential synthesis approach.

Two important linear programming (LP) models for the minimum utility cost target are the transportation (Cerda et al., 1983) and transhipment models (Papoulias and Grossmann, 1983). The transportation model incorporates match restrictions, multiple utilities and utilities available over a range of temperatures in the formulation (Cerda et al., 1983); while the transhipment model can handle unrestricted and restricted matches as well as identify the pinch point of the problem (Papoulias and Grossmann, 1983). Ježowski and Friedler (1992) extended the transhipment model (Papoulias and Grossmann, 1983) for multiple utilities and forbidden matches. Furthermore, the authors extended the dual temperature approach method (an insight-based approach) for problems with forbidden matches to further enhance energy recovery in the HEN. On the other hand, Galli and Cerda formulated mixed integer linear programming (MILP) (Galli and Cerda, 1998b; Galli and Cerda, 1998c) and MINLP (Galli and Cerda, 1998a) models that allow additional structural constraints in targeting for minimum utility cost.

In many process synthesis and optimisation problems, flowrates and temperatures of the process streams are unknown variables, as they are results of an optimal network. Therefore, when heat exchanger network (HEN) is taken into account during a flowsheet synthesis problem, the synthesis problem becomes very challenging due to the strong interaction between the process flowsheet and HEN. Hence, the conventional practise is to adopt the sequential approach where the non-integrated process flowsheet is first synthesised (in which flowrates and temperatures of the process streams are determined); followed by heat exchanger network synthesis. However, this approach may not achieve an overall optimum design, as it does not take in account trade-off between the process flowsheet and HEN.

To overcome this limitation Duran and Grossmann (1986) established a simultaneous approach with proper economic trade-off between process flowsheet and HEN, where flowrates and temperatures of process streams are the optimisation variables. In this work, the authors initiated the floating pinch approach for HEN utility targeting. The basic idea of floating pinch is to postulate a set of pinch point candidates based on the inlet temperatures of the hot and cold streams. Constraints are then developed for each of the postulated pinch point candidates, which will then identify the true pinch point and also the minimum hot and cold utilities. The main drawback of this approach is that, maximum operators are used to parameterise the stream locations. This causes non-differentiability in the mathematical program and thus a special non-smooth optimisation algorithm is required to solve it.

2.2.2 Resource conservation networks

One of the most established areas in process integration is RCNs. A particular application with extensive works reported is the synthesis of water network. Similar to other resource conservation network (RCN) problems, synthesis of water network can be classified into two main approaches, namely, insight-based and mathematical optimisation approaches. These two techniques complement each other well. The former technique divides the synthesis task into a two-step procedure, i.e. utility targeting and network design. The main strengths of the insight-based techniques are the ability to set rigorous network targets ahead of detailed RCN design, and to provide good insights for process designers. On the other hand, mathematical optimisation approaches do not provide as much as good insights for process designers, instead, they can generally handle more complex problems, such as multiple-contaminant systems, compulsory/forbidden matches between process operations, etc.

Insight-based approaches for water network synthesis were first reported by Smith and co-workers for reuse and regeneration systems (Wang and Smith, 1994; Wang and Smith, 1995; Kuo and Smith, 1998). Other works on regeneration systems were also reported (Bai et al., 2007; Feng et al., 2007). However, these works were limited to *fixed load problem*. Various works for more generalised *fixed flowrate problem* were also reported for direct reuse/recycle (Dhole et al., 1996; Polley and Polley, 2000; Hallale, 2002; El-Halwagi et al., 2003; Manan et al., 2004; Prakash and Shenoy, 2005; Bandyopadhyay et al., 2006; Foo et al., 2006b; Almutlaq and El-Halwagi, 2007; Foo, 2007; Shenoy and Bandyopadhyay, 2007; Foo, 2008) and for regeneration systems (Ng et al., 2007a; Ng et al., 2008b). Furthermore, the use of combined conceptual-based and mathematical optimisation techniques was also reported for water network synthesis with reuse/recycle, regeneration and total water network (Alva-Argáez et al., 2007; Ng et al., 2007b; Ng et al., 2007c; Ng et al., 2009a; Ng et al., 2009b; Ng et al., 2010). Note that total water network consists of the elements of water reuse/recycle, regeneration (treatment for reuse/recycle), and waste treatment (treatment for final discharge).

On the other hand, Takama and co-workers (Takama et al., 1980b; Takama et al., 1980a) initiated mathematical optimisation approaches for water network synthesis. Various mathematical optimisation works on synthesis of water network have been presented at later stage, which may be further categorised as direct reuse/recycle (Bagajewicz et al., 2000; Savelski and Bagajewicz, 2000; Yang et al., 2000; Bagajewicz and Savelski, 2001; Gomez et al., 2001; Savelski and Bagajewicz, 2001; Savelski and Bagajewicz, 2003; Tan and Cruz, 2004; Karuppiah and Grossmann, 2006; Alva-Argáez et al., 2007) and regeneration systems (Gabriel and El-Halwagi, 2005; Karuppiah and Grossmann, 2006; Khor et al., 2011). Reviews on various techniques in water network synthesis problem can be found in literature (Bagajewicz et al., 2000; Smith, 2005; El-Halwagi, 2006; Ježowski, 2010; Foo, 2012).

From the above discussion, it is observed that the techniques developed for RCN is rather well established. However, the major drawback of the previous works is that, they are limited to "chemo-centric" problems (Shelley and El-Halwagi, 2000; El-Halwagi, 2006), where chemical concentration is the main factor for consideration in performing material recovery. However, note that many design problems are not limited by the nature and quantity of chemical of the streams. Other properties or functionalities of streams (e.g. pH, density, colour, etc.) are also equally important (El-Halwagi, 2006; Foo, 2012). Furthermore, the effluent regulation is commonly defined not only in term of pollutant concentration but also based on stream properties, such as pH, colour, etc. To overcome this limitation, El-Halwagi and co-workers (Shelley and El-Halwagi, 2000; El-Halwagi et al., 2004) introduced the notion of property integration. Since then, various methodologies have also been established for the design of property-based RCN.

Shelley and El-Halwagi (2000) introduced the concept of property-based cluster that is able to track functionalities and properties of streams instead of their chemical constituents. This technique was established to recover and allocate volatile organic compounds (VOCs) in complex hydrocarbon mixtures. For RCNs that consider up to three properties, graphical tool may be utilised to assist the synthesis and analysis tasks (Shelley and El-Halwagi, 2000; El-Halwagi et al., 2004). On the other hand, (Qin et al., 2004) developed algebraic tools for processes involving more than three properties.

Kazantzi and El-Halwagi (2005) and Foo et al. (2006a) extended the conventional targeting techniques developed for concentration-based RCN into property integration problem. Besides, Ng and co-workers extended their automated targeting techniques (Ng et al., 2009a; Ng et al., 2009b) for property-based RCN problems too (Ng et al., 2009c; Ng et al., 2010). Concurrently, there is also a small group of methods that focus on batch processes (Grooms et al., 2005; Ng et al., 2008a; Chen et al., 2010).

Moreover, some works have also been extended to simultaneous mass and property integration. Ponce-Ortega et al. (2009) presented mathematical models to simutaneously optimise the concentration- and property-based RCNs which satisfy both the process and environmental constraints. An MINLP formulation with waste treatment system was proposed. The model is based on disjunctive programming and takes into consideration of technologies in wastewater treatment. In addition, Ponce-Ortega et al. (2010) developed a mathematical model based for concentration- and property-based RCNs with interception network. The model excludes most of the non-linearities of the system with the remaining bilinear terms that are handled with a relaxation approach in order to yield a global optimal solution.

On the other hand, an alternative property-based RCNs model with recovery and treatment systems was presented by Hortua et al. (2012). The recovery system is used to recover valuable materials as byproducts while treatment system is include to ensure that the waste disharge complies with environmental regulations. The proposed model determines the minimum total cost which consists of the operational cost of fresh resources, material recovery and waste treatment, and the annualised piping and capital cost. Furthermore, in the model, the recovery system is only utilised when the concentration of the valuable materials reaches the minimum value to ensure that it is worth investing on the recovery system. However, these works in the area of mass and property integration do not consider heat effect in their problem formulation.

Recently, Kheireddine et al. (2011) further extended the area of mass and property integration with thermal constraints. In this work, a nonlinear programming (NLP) model that minimises the total annualised cost of direct reuse/recycle network to satisfy a set process and environmental constraints is presented. Furthermore, the model also accounts for heat of mixing and the inter-dependence of properties. However, the main drawback of this proposed model is that, it involves direct mixing without heat integration. In some cases, when the thermal constraints are unable to be satisfied through direct mixing, external heating and cooling utilities should be considered.

2.2.3 Heat integrated water networks

Over the past decades, synthesis of HIWNs has received particular attention and many studies have been conducted. Salveski and Bagajewicz (1997) considered water and energy consumptions separately, and solving the problem in a sequential manner. Later, both insight-based and mathematical optimisation techniques have been established. Note that the insight-based techniques are developed based on sequential approach. Meanwhile, both sequential and simultaneous approaches can be considered in mathematical optimisation techniques.

As reported in the literature, the currently available insight-based techniques include two dimensional grid diagram with separate systems (Savulescu et al., 2005b; Savulescu et al., 2005a; Leewongtanawit and Kim, 2009), source-demand energy composite curves (Savulescu et al., 2002; Manan et al., 2009; Alwi et al., 2011), stream merging principles (Feng et al., 2008), graphical thermodynamic rules (Sorin and Savulescu, 2004; Thomas Polley et al., 2010), energy recovery algorithm (Sahu and Bandyopadhyay, 2010), modified problem table algorithm (Bandyopadhyay and Saha, 2010) and temperature versus concentration diagram (Martínez-Patiño et al., 2011). However, these methods are limited to single contaminant problems.

To address multiple contaminants measurements, mathematical programming techniques have been proposed. Sequential linear programming models have been developed to first determine the minimum fresh water consumption followed by minimum energy requirement (Bagajewicz et al., 2002; Feng et al., 2009; George et al., 2011; Sahu and Bandyopadhyay, 2012). Detailed heat integrated water network (HIWN) is then identified via MINLP models (Bagajewicz et al., 2002; Feng et al., 2009; George et al., 2011; Sahu and Bandyopadhyay, 2012).

Bagajewicz et al. (2002) initiated the sequential approach for the synthesis of heat integrated water network (HIWNs). The fresh water and energy targets are firstly achieved using a LP formulation based on the necessary conditions of optimality. In the second stage, an MINLP heat transhipment model is generated. These models incorporate non-isothermal mixing as well as forbidden and compulsory flow connections and heat transfer matches.

Feng et al. (2009) analysed the interconnections between the design of a water allocation network and the design of a heat exchanger network. The authors discovered that reducing the number of temperature local fluctuations along the sub-streams in water networks improves the energy performance of the system. As a result, mathematical model with this consideration was proposed to synthesise a HIWN.

The work by Bagajewicz et al. (2002) and Feng et al. (2009) are primarily applicable to *fixed load problems*. To overcome this limitation, George et al. (2011) established a sequential approach for the *fixed flowrate problems*. The methodology is demonstrated with both single and multiple contaminants with the incorporation of isothermal and non-isothermal mixing of streams. A linear programming model is formulated to identify the fresh water target. For HEN, a linear transshipment model is formulated for isothermal mixing problem while a nonlinear programming model with a discontinuous derivative is formulated for non-isothermal mixing cases.

Liao et al. (2011) developed an approach for HIWNs that allow operation split. Firstly, utility targets and operation split conditions are first obtained. Next, an MINLP model is initiated to achieve the desired water network design and heat exchanger network design. However, the authors separate the direct and indirect heat transfer in the targeting stage.

Recently, Sahu and Bandyopadhyay (2012) extended the concept of modified problem table algorithm (Sahu and Bandyopadhyay, 2010) to formulate HIWNs as linear programming model. The authors formulated three LP models for targeting the fresh water and energy consumptions for isothermal and non-isothermal mixing situations. The proposed formulation avoids the sub-optimality issue of MINLP and discontinuous nonlinear programming (DNLP) formulations. However, iteration of different pinch points is needed to identify the minimum energy requirement.

On the other hand, the total cost of HIWNs is minimised with simultaneous techniques. Leewongtanawit and Kim (2008) initiated mathematical models for synthesis of HIWNs with multiple contaminants. The authors formulate the overall problem as an MINLP optimisation problem. Next, a decomposition approach is introduced to decompose the overall MINLP problem into MILP and NLP sub-problems which are solved in sequence using an iterative process. The method has also considered a trade-off between water network and HEN, non-isothermal and generation of separate systems. Another MINLP model for HIWNs synthesis has been determined by Bogataj and Bagajewicz (2008). The established model includes the NLP formulation of water network superstructure and the MINLP formulation of heat exchange network superstructure for non-isothermal stream mixing.

The models presented by Leewongtanawit and Kim (2008) and Bogataj and Bagajewicz (2008) utilised heuristics to reduce the number of hot and cold streams in the HEN, which had reduced the size of the model. However, the limitation of these approaches is that, they might exclude the potential promising HIWNs. As a result, Dong et al. (2008) modify the state-space superstructure to formulate an MINLP model which covers a broader network structures. However, the model is very large in size and it is computational expensive when the problem scale increases. As a result, an integrated optimisation strategy has been established to improve the solution quality and efficiency. The potential global optimum may be identified by applying an interaction method proposed.

Ataei and Yoo (2010) proposed a sequential approach for multiple contaminant systems with the consideration of flowrate changes and heat loss in the HIWNs. Firstly, an NLP model is established to identify the feasible non-isothermal mixing points that provide the overall network with minimum fresh water and energy consumptions. Next, HEN is simplified through a new generation of separate system in HEN.

2.3 The research gap

From the above review, it is observed that the current HIRCNs work mainly focus on HIWNs problems. However, no work on property-based HIRCNs has been developed. Therefore, a generic methodology for concentration- and property-based HIRCNs is yet to be established.

The main challenge of this generic methodology is to considered mass and property integration together with heat integration, in order to achieve minimum cost for fresh resources and hot and cold utilities. With this methodology established, resource and energy conservation objectives can be achieved simultaneously. Besides, this methodology plays an important role as both material and energy resources are equally important in the process industries. Moreover, property of resources may be temperature-dependent in some cases; hence property and heat recovery should be addressed together.

CHAPTER 3: OVERALL METHODOLOGY DEVELOPMENT

3.1 Introduction

As shown in Chapter 2, extensive works have been reported on concentration-based heat integrated resource conservation networks (HIRCNs), and more specifically on heat integrated water networks (HIWNs). However, these methods are not applicable directly for property-based HIRCNs as they are essentially "chemo-centric". Therefore, a more generic approach for the synthesis of concentration- and property-based HIRCNs is needed. This can be achieved via the integration of concentration- and property-based resource conservation networks (RCNs) with heat exchanger networks (HENs). This chapter mainly focuses on the overall methodology development for concentration- and property-based HIRCNs, and a general framework for the synthesis of HIRCNs with and without the consideration of heat of mixing.

3.2 Overall methodology development

An overall methodology for the synthesis of concentration- and property-based HIRCNs is developed and shown in Figure 3.1. Firstly, limiting data for process sources and sinks (which includes flowrate, temperature and other important stream properties) are extracted for the desired case study.

Next, one needs to evaluate if heat of mixing is to be considered for a case study. Heat of mixing represents how systems of gases or liquids undergo temperature change as a result of energy generation (exothermic mixing) or absorption (endothermic mixing) during the mixing processes. The evaluation needs to be conducted based on the type of mixtures in the process streams for a given system. When liquid is involved in the process streams (i.e. gas-liquid mixture, liquid-liquid mixture or liquid-solid mixture), heat of mixing should be considered. On the other hand, heat of mixing can be ignored in situations with gas-gas mixture, gas-solid mixture and solid-solid mixture, or with dilute liquid systems, as they are negligible.

Once decision is made on the heat of mixing, the case study may be solved using the model presented by Kheireddine et al. (2011) where no heat exchanger network (HEN) is involved. Note that this model is useful for solving RCN without HEN, with and without heat of mixing. If an optimal solution is attained, this means that the case study does not need HEN with external energy utilities, as the thermal constraints of the process sinks are satisfied through direct mixing of the process sources. Therefore, HEN is not needed and the optimal solution has been found. However, when no feasible solution can be achieved, one will then proceed to the HIRCNs model presented in this thesis.

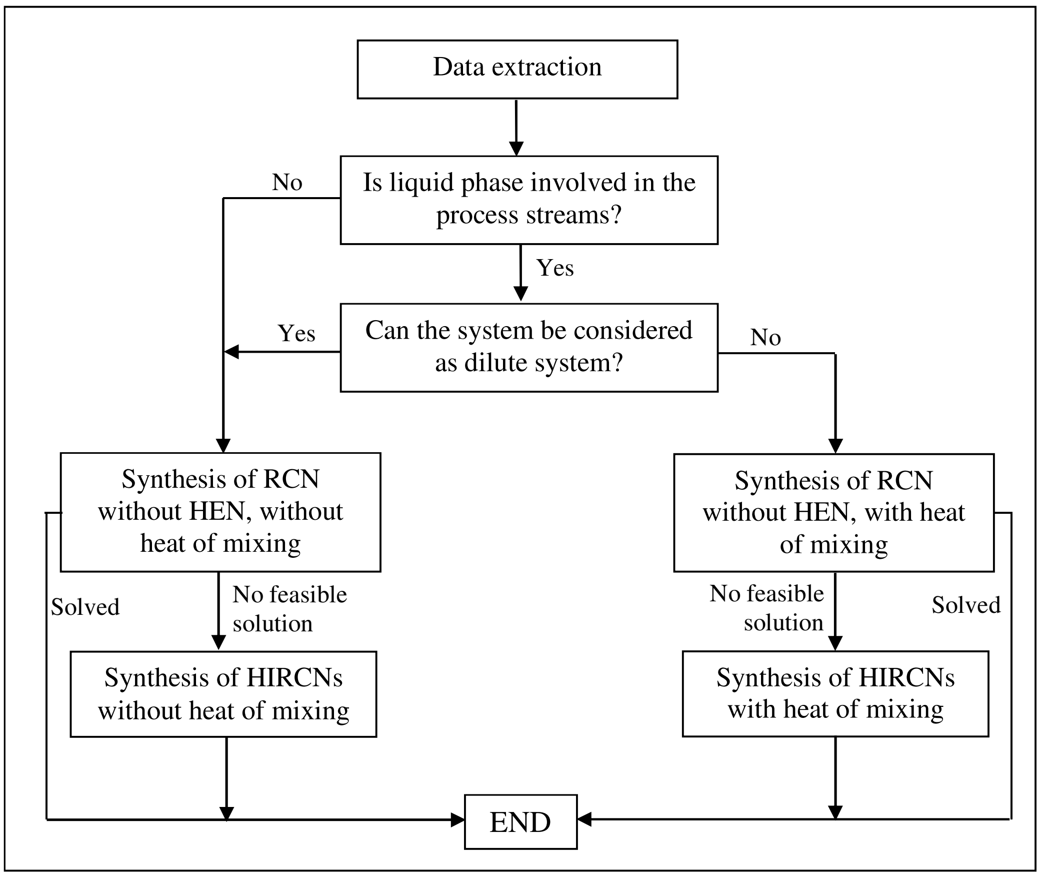


Figure 3.1: Overall methodology development for the synthesis of concentration- and property-based HIRCN.

3.2.1 Case studies

Four case studies are used to illustrate the proposed overall methodology. All cases are solved using Extended LINGO v13.0 with Global Solver in a computer with a Core i3, 3.3 GHz processor.

3.2.1.1 Case study 1

Case study 1 is an ammonia recovery case study taken from Sahu and Bandyopadhyay (2012). It involves a process plant that utilises ammonia as the mass separating agent in a sour gas absorption column and as a dust-cleaning agent. On the other hand, ammonia waste is produced in the calcium chloride production section of the plant, which is currently sent to waste treatment system. Therefore, to reduce the waste generation, ammonia can be recovered to process units which require ammonia. The limiting data for this case study is showed in Table 3.1.

Table 3.1: Process limiting data for Case study 1.

Sink	Flowrate (kg/s)	Temperature (^{o}C)	Concentration (ppm)
SK1	350	30	0
SK2	677	187	40
SK3	126	55	75
SK4	202	98	100
Source	**Flowrate (kg/s)**	**Temperature (^{o}C)**	**Concentration (ppm)**
SR1	530	21	30
SR2	68	43	150
SR3	1130	130	300
SR4	36	35	500

With the limiting data obtained, evaluation is then conducted on whether heat of mixing should be considered in this case study. Ammonia that is to be recovered in this case study appears to be in gas phase in the process streams with hydrogen sulfide. Therefore, no liquid is involved in the process streams. Based on the proposed overall methodology, heat of mixing is not to be included in this case study as it is negligible for gas-gas mixture. Next, the case study is solved using the model presented by Kheireddine et al. (2011) where no HEN is involved. As no feasible solution is obtained, this case study will need to be solved using the methodology for HIRCNs synthesis without heat of mixing presented in Chapter 5.

3.2.1.2 Case study 2

Case study 2 is adapted from Nápoles-Rivera et al. (2010), where multiple properties are considered, i.e. concentration, toxicity, theoretical oxygen demand (THOD), pH, density, viscosity and temperature. The lower and upper bound constraints on concentration, toxicity, THOD, pH, density, viscosity and temperature ensure that the operational conditions of the sinks are to be fulfilled. Table 3.2 shows the limiting data for process sinks and sources for this case study.

The resource to be recovered in this case study is water which means that liquid phase occurs in the process streams. However, based on the limiting data shown in Table 3.2, this case study can be considered as a dilute system because the concentration of the process sources and sinks in the limiting data are low (ranging from 0 ppm to 0.033 ppm which it is below 0.000000033 mass fraction). Therefore, heat of mixing can be ignored in this case study. When this case study is solved without heat of mixing using the model by Kheireddine et al. (2011), no feasible solution is obtained. As a result, the HIRCNs without heat of mixing methodology presented in Chapter 5 is needed to obtain the HIRCNs for this case study.

3.2.1.3 Case study 3

Case study 3 reports a single property-based water network adopted from George et al. (2011). It consists of three process sinks and three process sources, with acetone and water in the process streams. The limiting data for this case study is given in Table 3.3.

Table 3.2: Process limiting data for Case study 2.

Sink	Flowrate (lb/h)	Concentration (ppm)	Toxicity (%)	THOD (mg O2/l)	pH	Density (lb/l)	Viscosity (cP)	Temperature (°C)
SK1	3000	0 – 0.013	0 - 2	0 - 75	5.9 – 8.0	1.8 – 2.8	0.871 – 1.202	130 – 180
SK2	1900	0 – 0.011	0 - 2	0 - 75	5.7 – 7.9	1.7 – 2.5	0.782 – 1.430	60 - 110
Waste	-	-	-	-	-	-	-	27 - 35
Source	**Flowrate (lb/h)**	**Concentration (ppm)**	**Toxicity (%)**	**THOD (mg O2/l)**	**pH**	**Density (lb/l)**	**Viscosity (cP)**	**Temperature (°C)**
SR1	2900	0.033	0.8	75	5.3	2.000	1.256	160
SR2	2450	0.022	0.5	88	5.1	2.208	1.220	120
Fresh	-	0	0	0	7.0	2.204	1.002	25

The process streams in Case study 3 involve liquid phase due to the presence of water. The concentration level of the limiting data range from 0 ppm to 1100 ppm (equal to 0.0011 mass fraction). Thus, this is not a dilute system and heat of mixing should be considered. Furthermore, this case study will be proceed to the HIRCNs with heat of mixing methodology presented in Chapter 6 as no feasible solution is found when it is solved using the model by Kheireddine et al. (2011).

Table 3.3: Process limiting data for Case study 3

Sink	Flowrate, F (kg/s)	Temperature, T ($^{\circ}$C)	Concentration, C (ppm)
SK1	100	100	50
SK2	40	75	50
SK3	166.67	100	800
Wastewater (WW)	-	30	-
Source	**Flowrate, F (kg/s)**	**Temperature, T ($^{\circ}$C)**	**Concentration, C (ppm)**
SR1	100	100	100
SR2	40	75	800
SR3	166.67	100	1100
Fresh water (FW1)	-	20	0

3.2.1.4 Case study 4

Case study 4 is adapted from Kheireddine et al. (2011) and only involves phenol and water in the process streams. Multiple properties (concentration, temperature and vapour pressure) are considered. Note that the heat capacities in this case study are interdependence of temperature effect. Table 3.4 shows the limiting data for process sinks and sources as well as fresh resources for this case study.

Table 3.4: Process limiting data for Case study 4.

Sink	Flowrate (kg/hr)	Minimum temperature (°C)	Maximum temperature (°C)	Minimum vapour pressure (kPa)	Maximum vapour pressure (kPa)	Minimum concentration (mass fraction)	Maximum concentration (mass fraction)
SK1	2718	70	85	15	35	0	0.013
SK2	1993	30	50	10	25	0	0.013
SK3	1127	25	65	13	40	0	0.1
Source	**Flowrate (kg/hr)**	**Temperature (°C)**		**Vapor pressure (kPa)**		**Concentration (mass fraction)**	
SR1	3661	75		38		0.016	
SR2	1766	65		25		0.024	
SR3	1485	40		7		0.22	
FR1	-	25		3		0	
FR2	-	35		6		0.012	

Heat of mixing is considered in Case study 4 as liquid phase is involved in the process streams due to the presence of water. Besides, the concentration of the limiting data ranges from 0 to 0.22 mass fraction (equal to 220,000 ppm) which is considered high concentration. Due to changes in limiting data as compared to the original data from Kheireddine et al. (2011), infeasible solution occurred when the case study is solved by using Kheireddine et al. (2011) model. Consequently, methodology for HIRCNs with heat of mixing in Chapter 6 can be used to achieve the desired HIRCNs.

3.3 Framework for the synthesis of HIRCNs with and without heat of mixing

A general framework is established to synthesise concentration- and property-based HIRCNs with and without consideration of heat of mixing. This section presents the outline of such strategy. As indicated in Figure 3.2, the suggested procedure for both synthesis of HIRCN with and without heat of mixing involves the following steps:

1. Problem statement formulation.
2. A source-HEN-sink superstructure is derived to identify the stream connection between process sources and sinks, as well as the placement of HEN.
3. The proposed source-HEN-sink superstructure is formulated as a mixed integer nonlinear programming (MINLP) problem which has the objective to minimise the total cost. The model can be sub-divided into concentration- and property-based RCNs, and HENs models. The RCNs model is mainly based on flowrate, energy and property operator balances for process sinks and sources while the HENs model is adapted from the revised HEN floating pinch approach in this work.
4. A solution strategy is developed to achieve the desired HIRCN solution.
5. The HIRCN configuration is drawn based on the solution obtained. Furthermore, the HEN design is synthesised using the classical *pinch design method* (Linnhoff et al., 1982; Smith, 2005) in order to verify the targeted results of hot and cold utilities in the solution.

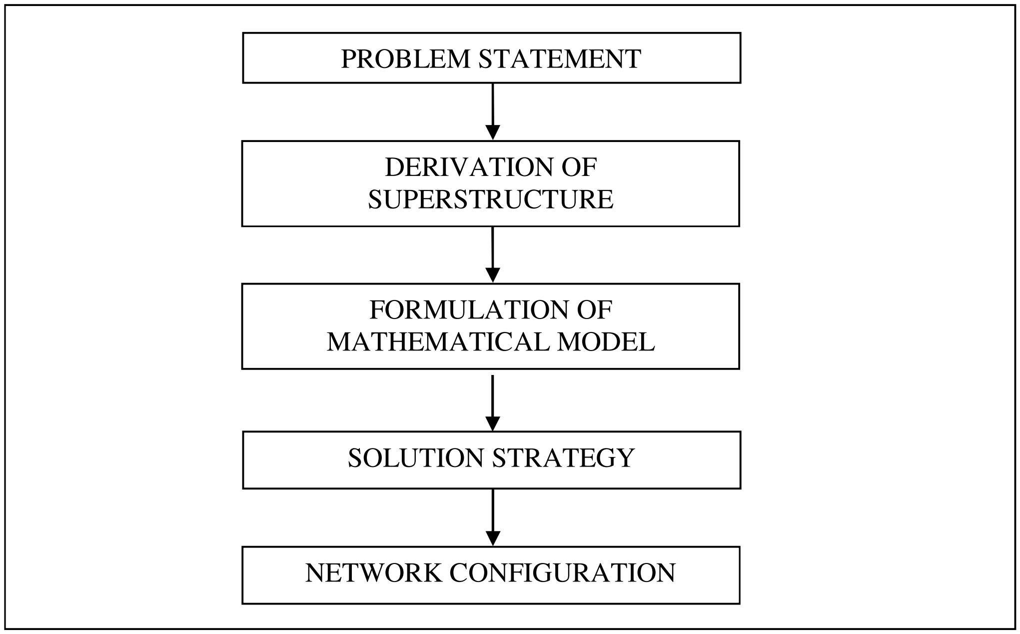


Figure 3.2: General framework for the synthesis of HIRCNs with and without heat of mixing

3.4 Chapter summary

In this chapter, a generic overall methodology for concentration- and property-based HIRCNs has been proposed. This methodology provides the overall process on the selection of HIRCNs without and with heat of mixing. Four case studies are solved to illustrate this proposed methodology. The latter part of this chapter presents a general framework to synthesis HIRCNs that can be applied to both without and with heat of mixing situations. The detailed synthesis methodology will be addressed in the subsequent chapters of this thesis.

CHAPTER 4: FLOATING PINCH METHOD FOR HEAT EXCHANGER NETWORK

4.1 Introduction

A general formulation of resource conservation network (RCN) problems consists of varying process parameters such as flowrates, temperatures, and properties. Thus, in heat integrated resource conservation network (HIRCN) problems, the flowrates and temperatures of the heat exchanger network (HEN) are also varied. However, the established HEN models for fixed stream conditions, such as problem table (Linnhoff and Flower, 1978a), transportation problem (Cerda et al., 1983) and transshipment model (Papoulias and Grossmann, 1983), cannot be applied in this case. Therefore, the floating pinch method established by Duran and Grossmann (1986) need to be incorporated. Nevertheless, in this method (Duran and Grossmann, 1986), maximum operators are used to parameterise the hot and cold stream locations in the composite curves. This causes non-differentiability in the mathematical program which can only be solved via a special non-smooth optimisation algorithm. To overcome this limitation, this work extends the floating pinch method for mass exchange network by El-Halwagi and Manousiouthakis (1990) which uses binary variables to parameterise the stream locations to HEN. This chapter presents the revised HEN floating pinch method.

4.2 Problem statement

The problem addressed in this chapter is stated as follows:

Given *NHOT* of hot streams that need to be cooled and *NCOLD* of cold streams that need to be heated. Each hot stream *h* and cold stream *c* has fixed or acceptable range of flowrate, supply and target temperature, given as in Equations 4.1 – 4.6.

$$m_h^{\min} \leq m_h \leq m_h^{\max} \quad h \in NHOT \tag{4.1}$$

$$m_c^{\min} \le m_c \le m_c^{\max} \;\; c \in NCOLD \tag{4.2}$$

$$T_h^{\text{in,min}} \le T_h^{\text{in}} \le T_h^{\text{in,max}} \;\; h \in NHOT \tag{4.3}$$

$$T_c^{\text{in,min}} \le T_c^{\text{in}} \le T_c^{\text{in,max}} \;\; c \in NCOLD \tag{4.4}$$

$$T_h^{\text{out,min}} \le T_h^{\text{out}} \le T_h^{\text{out,max}} \;\; h \in NHOT \tag{4.5}$$

$$T_c^{\text{out,min}} \le T_c^{\text{out}} \le T_c^{\text{out,max}} \;\; c \in NCOLD \tag{4.6}$$

where $m_h^{\min}$, $m_h^{\max}$, $m_c^{\min}$ and $m_c^{\max}$ are the respective lower and upper bounds of the allowable specific heat capacity flowrate for hot stream *h* and cold stream *c*, while $T_h^{\text{in,min}}$, $T_h^{\text{in,max}}$, $T_c^{\text{in,min}}$, $T_c^{\text{in,max}}$, $T_h^{\text{out,min}}$, $T_h^{\text{out,max}}$, $T_c^{\text{out,min}}$ and $T_c^{\text{out,max}}$ refer to the lower and upper bounds of the supply and target temperature for hot stream *h* and cold stream *c* respectively. The heat capacity for each hot stream *h* and cold stream *c* can be either constant or temperature dependence. In addition, external hot (Q_h) and cold (Q_c) utilities are available to fulfill the process requirement after energy recovery between the hot and cold streams is maximised. The overall objective is to locate the minimum hot and cold utility targets in a HEN.

4.3 Concept of HEN floating pinch method

To understand the concept of floating pinch method, an understanding of the heat transfer composite curves is needed. As shown in Figure 4.1(a), the hot and cold composite curves are merged by individual streams via linear superposition, and plotted on a temperature versus enthalpy diagram. These curves are then brought together via horizontal displacement until they reached a minimum temperature difference ($\Delta T_{\min}$). The vertical overlapping region between the two composite curves shows the energy recovery from the hot streams to the cold streams (Smith, 2005).

If both composite curves are shifted vertically (i.e. hot composite curve is $\Delta T_{min}/2$ cooler; and cold composite is $\Delta T_{min}/2$ hotter) until they touch at the true pinch point, as shown in Figure 4.1(b), one can observe the following:

1. The potential pinch candidate(s) are those corner points on the composite curves, that correspond to the inlet temperatures of any hot and cold streams (Duran and Grossmann, 1986).

2. The total energy balance for the HEN must always be achieved (total heat removal of the hot streams and that supplied by the external hot utility should be equal to the total heat gained by the cold streams and that of external cold utility). To minimise the external hot and cold utilities, no energy should be transferred across the pinch (Smith, 2005). Hence, the true pinch point divides the composite curves into two regions, a heat source and a heat sink. The energy balance for both regions must also be satisfied.

3. To ensure feasible heat transfer, the hot composite curve must always stay above the cold composite curve, with both composite curves touching only at the true pinch point.

4. If the composite curves touch at any potential pinch candidates other than the true pinch point (Figure 4.1(c)), some portions of the hot composite curve may lie below the cold composite curve in the same temperature range. For such situation, energy transfer between the composite curves is thermodynamically infeasible.

The basic idea of floating pinch is to postulate a set of pinch point candidates based on the inlet temperatures of the hot and cold streams. Constraints are then developed for each of the postulated pinch point candidates, which will then identify the true pinch point and also the minimum hot and cold utilities. The following section presents the HEN model of the HIRCN, with the adoption of the floating pinch concept.

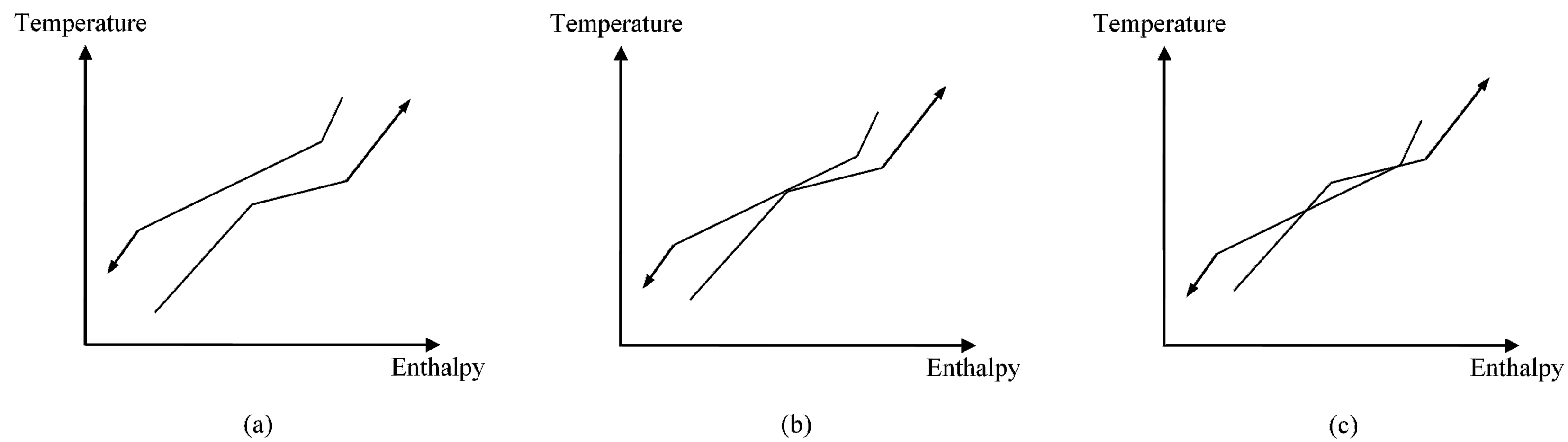


Figure 4.1: (a) Hot and cold composite curves. (b) Shifted hot and cold composite curves at true pinch point. (c) Infeasible hot and cold composite curves.

4.4 Mathematical model for HEN floating pinch

The revised HEN floating pinch based mathematical model is developed based on the HEN floating pinch concept explained in Section 4.3. The supply and target temperatures of the hot and cold streams from fresh resource *r* and source *i* to sink *j* are first shifted by subtracting $\Delta T_{\min}/2$ for hot streams; while adding $\Delta T_{\min}/2$ for cold streams. These temperatures are given by the equations as follows,

$$T_h^{\mathrm{s}} = T_h^{\mathrm{in}} - \frac{\Delta T_{\min}}{2} \tag{4.7}$$

$$T_h^{\mathrm{t}} = T_h^{\mathrm{out}} - \frac{\Delta T_{\min}}{2} \tag{4.8}$$

$$T_c^{\mathrm{s}} = T_c^{\mathrm{in}} + \frac{\Delta T_{\min}}{2} \tag{4.9}$$

$$T_c^{\mathrm{s}} = T_c^{\mathrm{out}} + \frac{\Delta T_{\min}}{2} \tag{4.10}$$

where T_h^{in}, T_h^{out}, T_c^{in} and T_c^{out} are the actual supply and target temperatures of the hot and cold streams, while T_h^{s}, T_h^{t}, T_c^{s} and T_c^{t} are the shifted supply and target temperatures of the hot and cold streams in HEN respectively. Note that Equations 4.7 – 4.10 may varies depending on the superstructure of HIRCN derived.

The potential pinch candidate, T_q corresponds to the inlet temperatures of the hot and cold streams (Duran and Grossmann, 1986),

$$T_q = \begin{bmatrix} T_h^{\mathrm{s}} \\ T_c^{\mathrm{s}} \end{bmatrix} \quad \begin{array}{l} h \in NHOT \\ c \in NCOLD \\ q \in NPINCH \end{array} \tag{4.11}$$

To identify the true pinch point and to ensure thermodynamic feasibility, the total energy balance is to be used together with energy balance above or below the pinch point candidates. Stream location parameterisation is needed in order to determine the energy balance above or below the pinch point candidates. In the floating pinch approach for HEN presented by Duran and Grossmann (1986), the authors used maximum operators to parameterise the stream locations. However, this approach causes non-differentiability in the mathematical program and thus a special non-smooth optimisation algorithm is required to solve it. In this work, binary variables are used to parameterise the stream locations, following the floating pinch method for mass exchange network (El-Halwagi and Manousiouthakis, 1990).

The binary variables used to parameterise the stream locations in order to determine the energy balance above the pinch point candidates are given by the constraints in Equations 4.12 – 4.15.

$$\beta^{t}_{h,q} = \begin{cases} 1 \ \ if \ T^{t}_{h} > T_q & h \in NHOT \\ 0 \ \ if \ T^{t}_{h} \le T_q & q \in NPINCH \end{cases} \tag{4.12}$$

$$\beta^{s}_{h,q} = \begin{cases} 1 \ \ if \ T^{s}_{h} > T_q & h \in NHOT \\ 0 \ \ if \ T^{s}_{h} \le T_q & q \in NPINCH \end{cases} \tag{4.13}$$

$$\gamma^{t}_{c,q} = \begin{cases} 1 \ \ if \ T^{t}_{c} > T_q & c \in NCOLD \\ 0 \ \ if \ T^{t}_{c} \le T_q & q \in NPINCH \end{cases} \tag{4.14}$$

$$\gamma^{s}_{c,q} = \begin{cases} 1 \ \ if \ T^{s}_{c} > T_q & c \in NCOLD \\ 0 \ \ if \ T^{s}_{c} \le T_q & q \in NPINCH \end{cases} \tag{4.15}$$

where $\beta^{t}_{h,q}, \beta^{s}_{h,q}, \gamma^{t}_{c,q}$ and $\gamma^{s}_{c,q}$ are the binary integer.

Equations 4.12 – 4.15 can be modelled using linear formulations as follow:

$$(L^{t}_{h} - T_q) * \beta^{t}_{h,q} < T^{t}_{h} - T_q \le (U^{t}_{h} - T_q) * (1 - \beta^{t}_{h,q}) \ \ h \in NHOT \ \ q \in NPINCH \tag{4.16}$$

$$(L^{s}_{h} - T_q) * \beta^{s}_{h,q} < T^{s}_{h} - T_q \le (U^{s}_{h} - T_q) * (1 - \beta^{s}_{h,q}) \ \ h \in NHOT \ \ q \in NPINCH \tag{4.17}$$

$$(L^{t}_{c} - T_q) * \gamma^{t}_{c,q} < T^{t}_{c} - T_q \le (U^{t}_{c} - T_q) * (1 - \gamma^{t}_{c,q}) \ \ c \in NCOLD \ \ q \in NPINCH \tag{4.18}$$

$$(L_c^s - T_q) * \gamma_{c,q}^s < T_c^s - T_q \le (U_c^s - T_q) * (1 - \gamma_{c,q}^s) \quad h \in NCOLD \quad q \in NPINCH \tag{4.19}$$

where L_h^t, L_h^s, L_c^t, L_c^s, U_h^t, U_h^s, U_c^t and U_c^s are the lower and upper bounds on the feasible values of T_h^t, T_h^s, T_c^t and T_c^s respectively.

The energy balance above the pinch point candidates is expressed as:

$$\begin{aligned} Q_h \ge & \sum_{c \in NCOLD} m_c CP_c \left\{ \gamma_{c,q}^s (T_q - T_c^s) - \gamma_{c,q}^t (T_q - T_c^t) \right\} - \\ & \sum_{h \in NHOT} m_h CP_h \left\{ \beta_{h,q}^t (T_q - T_h^t) - \beta_{h,q}^s (T_q - T_h^s) \right\} \quad q \in NPINCH \end{aligned} \tag{4.20}$$

where m_h, m_c, CP_h and CP_c are flowrate and specific heat capacity for hot stream h and cold stream c in HEN, respectively. Note that the second term shows the heat gained by cold stream c above the potential pinch point; while the third term of the equation shows the heat lost by hot stream h above a potential pinch candidate q.

Let us consider the following three cases where all possible locations of cold stream with respect to the pinch point are considered, to demonstrate how Equation 4.20 measures the energy above the pinch candidate.

1. Case 1 – cold stream c appears completely above the potential pinch point q. Equations 4.18 and 4.19 determine that integer $\gamma_{c,q}^s$ and $\gamma_{c,q}^t$ are equal to 1. Thus, heat load of cold stream c above the potential pinch point is given by $m_c CP_c \left\{ (T_q - T_c^s) - (T_q - T_c^t) \right\} = m_c CP_c (T_c^t - T_c^s)$.

2. Case 2 – cold stream c lies across a potential pinch point q as that T_c^s is below T_q while T_c^t is above T_q. Based on Equations 4.18 and 4.19, $\gamma_{c,q}^s = 0$ and $\gamma_{c,q}^t = 1$. Therefore, heat load of cold stream c above the potential pinch point is calculated by $m_c CP_c (T_c^t - T_q)$.

3. Case 3 – cold stream c appears completely below the potential pinch point q. Equations 4.18 and 4.19 define both $\gamma^{s}_{c,q}$ and $\gamma^{s}_{c,q}$ as zero. As a result, no heat is received by cold stream c above the potential pinch point.

Optionally, one can choose to use the energy balance below the pinch point candidate by using the constraints in Equations 4.21 - 4.24.

$$\lambda^{t}_{h,q} = \begin{cases} 1 \ \ if\ T^{t}_{h} < T_{q} & h \in NHOT \\ 0 \ \ if\ T^{t}_{h} \geq T_{q} & q \in NPINCH \end{cases} \tag{4.21}$$

$$\lambda^{s}_{h,q} = \begin{cases} 1 \ \ if\ T^{s}_{h} < T_{q} & h \in NHOT \\ 0 \ \ if\ T^{s}_{h} \geq T_{q} & q \in NPINCH \end{cases} \tag{4.22}$$

$$\eta^{t}_{c,q} = \begin{cases} 1 \ \ if\ T^{t}_{c} < T_{q} & c \in NCOLD \\ 0 \ \ if\ T^{t}_{c} \geq T_{q} & q \in NPINCH \end{cases} \tag{4.23}$$

$$\eta^{s}_{c,q} = \begin{cases} 1 \ \ if\ T^{s}_{c} < T_{q} & c \in NCOLD \\ 0 \ \ if\ T^{s}_{c} \geq T_{q} & q \in NPINCH \end{cases} \tag{4.24}$$

where $\lambda^{t}_{h,q}$, $\lambda^{s}_{h,q}$, $\eta^{t}_{c,q}$ and $\eta^{s}_{c,q}$ are the binary integer variables.

Equations 4.21 – 4.24 can be modelled using linear formulations as follow:

$$(L^{t}_{h} - T_{q}) * \lambda^{t}_{h,q} < T^{t}_{h} - T_{q} \leq (U^{t}_{h} - T_{q}) * (1 - \lambda^{t}_{h,q}) \ \ h \in NHOT \ \ q \in NPINCH \tag{4.25}$$

$$(L^{s}_{h} - T_{q}) * \lambda^{s}_{h,q} < T^{s}_{h} - T_{q} \leq (U^{s}_{h} - T_{q}) * (1 - \lambda^{s}_{h,q}) \ \ h \in NHOT \ \ q \in NPINCH \tag{4.26}$$

$$(L^{t}_{c} - T_{q}) * \eta^{t}_{c,q} < T^{t}_{c} - T_{q} \leq (U^{t}_{c} - T_{q}) * (1 - \eta^{t}_{c,q}) \ \ c \in NCOLD \ \ q \in NPINCH \tag{4.27}$$

$$(L^{s}_{c} - T_{q}) * \eta^{s}_{c,q} < T^{s}_{c} - T_{q} \leq (U^{s}_{c} - T_{q}) * (1 - \eta^{s}_{c,q}) \ \ h \in NCOLD \ \ q \in NPINCH \tag{4.28}$$

Equation 4.29 shows the energy balance below the pinch point candidate.

$$Q_c \geq \sum_{h \in NHOT} m_h CP_h \left\{ \lambda^{t}_{h,q}(T_q - T^{t}_h) - \lambda^{s}_{h,q}(T_q - T^{s}_h) \right\} - \sum_{c \in NCOLD} m_c CP_c \left\{ \eta^{s}_{c,q}(T_q - T^{s}_c) - \eta^{t}_{c,q}(T_q - T^{t}_c) \right\} \quad q \in NPINCH \tag{4.29}$$

To demonstrate the usefulness of Equation 4.29, let us consider the following situations where all possible locations of hot stream (with respect to the pinch point) are considered.

1. Case 1 – hot stream *h* lies completely above the potential pinch point *q*. Based on Equations 4.25 and 4.26, integer $\lambda^{s}_{h,q}$ and $\lambda^{t}_{h,q}$ are set to zero. Thus, heat lost by hot stream *h* below the potential pinch point is zero.

2. Case 2 – hot stream *h* appears completely below the potential pinch point *q*. Equations 4.25 and 4.26 next determine that $\lambda^{s}_{h,q} = \lambda^{t}_{h,q} = 1$. As a result, heat lost by hot stream *h* below the potential pinch point is given by Equation 4.29 that follows:

   $$m_h CP_h \left\{ (T_q - T^{t}_h) - (T_q - T^{s}_h) \right\} = m_h CP_h (T^{s}_h - T^{t}_h)$$

   which shows the correct expression.

3. Case 3 – hot stream *h* lies across a potential pinch point *q*, which means that T^{s}_h is above T_q while T^{t}_h is below T_q. Equations 4.25 and 4.26 determine that $\lambda^{s}_{h,q} = 0$ and $\lambda^{t}_{h,q} = 1$. Therefore, heat lost by hot stream *h* below the potential pinch point is given as $m_h CP_h (T_q - T^{t}_h)$.

The total energy balance is expressed as:

$$\sum_{h \in NHOT} m_h CP_h (T^{s}_h - T^{t}_h) - \sum_{c \in NCOLD} m_c CP_c (T^{t}_s - T^{s}_s) + Q_h - Q_c = 0 \tag{4.30}$$

To identify the minimum hot and cold utility targets for a given problem, one may make use of the total energy balance (Equation 4.30) together with the energy balance above the pinch point candidates (Equation 4.20; and its respective constraints in Equations 4.16 – 4.19). Alternatively, the total energy balance (Equation 4.30) may be used together with energy balance below the pinch point candidates (Equation 4.29, with its respective constraints in Equations 4.25 – 4.28).

To identify the true pinch point(s), one may make use of either Equations 4.20 (energy balance above the pinch point candidate(s)) or 4.29 (energy balance below the pinch point candidate(s)). For the case where Equation 4.20 is used, the difference between the second and third terms in this energy balance equation indicates the minimum hot utility that is needed for the HEN problem (Q_h). Hence, when a candidate is found to have the difference between the second and third terms (in Equation 4.20) matching the Q_h value reported by LINGO solution, this indicates that the candidate is the true pinch point of the HEN problem. Similarly, if Equation 4.29 is used, the difference between the second and third terms indicates the minimum cold utility (Q_c) for the HEN. Hence, the candidate(s) having the same value for the calculated difference that match Q_c value in the LINGO solution indicates that it is the true pinch point of the HEN problem. Note that the above formulation is MILP.

4.5 Case studies

To demonstrate the applicability of the HEN floating pinch model, two case studies are solved and presented in the following section. All case studies are solved using Extended LINGO v13.0 with Global Solver in a computer with a Core i3, 3.3 GHz processor and $\Delta T_{\min}$ is taken as 10°C.

4.5.1 Case study 5

Case study 5 is taken from Smith (2005), which consists of two hot streams and two cold streams. Table 4.1 shows the limiting data for this case study. The objective of this case study is to minimise the hot utility in HEN and is given as follows:

Table 4.1: Process limiting data for Case study 5.

Hot stream	Supply temperature (°C)	Target temperature (°C)	Heat capacity flowrate, $m_h \cdot CP_h$ (MW.K^{-1})
H1	250	40	0.15
H2	200	80	0.25
Cold stream	**Supply temperature (°C)**	**Target temperature (°C)**	**Heat capacity flowrate, $m_c \cdot CP_c$ (MW.K^{-1})**
C3	20	180	0.20
C4	140	230	0.30

4.5.2 Case study 6

Case study 6 involves a HEN problem for a process that involves phenol and water in the process streams. The limiting data is given in Table 4.2. Note that both hot and cold streams operate within a range of flowrates. To include the operating ranges in the model, additional constraints are added as follows:

$$10 \leq m_{h1} \leq 20 \tag{4.32}$$

$$10 \leq m_{h2} \leq 20 \tag{4.33}$$

$$5 \leq m_{c1} \leq 10 \tag{4.34}$$

$$15 \leq m_{c2} \leq 20 \tag{4.35}$$

Table 4.2: Process limiting data for Case study 6.

Stream	Supply temperature (°C)	Target temperature (°C)	Minimum flowrate, m^{min} (g/s)	Maximum flowrate, m^{max} (g/s)	Mole fraction of water	Mole fraction of phenol
H1	160	40	10	20	0.995	0.005
H2	80	60	10	20	0.998	0.002
C3	50	115	5	10	0.940	0.060
C4	80	220	15	20	0.978	0.022

All heat capacities of the process streams can be determined with Equation 4.36 (Shenoy, 1993):

$$CP = \sum x_k CP_k \quad k \in NCOMP \tag{4.36}$$

where x_k is the mole fraction of component k and heat capacity (CP) for each component can be determined using Equation 4.37 (Shenoy, 1993). Note that the heat capacity values are temperature-dependent.

$$CP_k = a_k + b_k T \quad k \in NCOMP \tag{4.37}$$

where a_k and b_k are parameters in linearised temperature-dependent expression for heat capacity of each component. Since this case study involves a binary system with phenol and water, a and b parameters for phenol are taken as 0.4685 J/(gK) and 0.0044 J/(gK) while a and b parameters for water are1.3724 J/(gK) and 0.0083 J/(gK) respectively. Note however that with the inclusion of Equation 4.37, the proposed model becomes an MINLP formulation.

In this case study, the same optimisation objective in Case study 5 is used. Equation 4.31 is solved subject to Equations 4.7 – 4.11, 4.25 – 4.30 and 4.32 – 4.37. The optimal solution achieved in 11 CPU seconds shows that the case study required Q_h, Q_c and true pinch points of 5.07 kW, 4.30 kW, 155ºC and 85ºC (multiple pinch) respectively. To further verify these results, the corresponding HEN that fulfils the targets is synthesised using the classical *pinch design method* (Linnhoff and Flower, 1978a; Linnhoff et al., 1982; Smith, 2005), and is presented in Figure 4.2. A total of six heat exchangers (three process to process heat exchangers, two coolers and one heater) are needed. Note that the energy targets are identical to those obtained via the proposed model. The LINGO code and solution for this case study can be found in Appendix B.

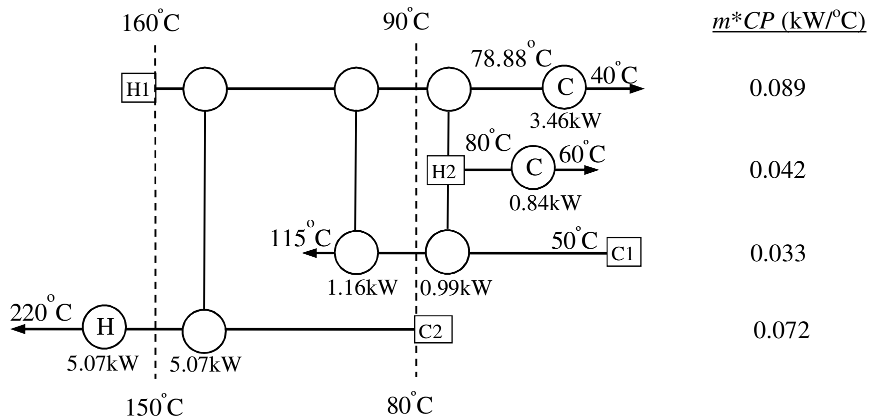


Figure 4.2: HEN for Case study 6.

4.6 Chapter summary

In this chapter, a new improved mathematical model has been developed for identifying minimum hot and cold utility targets for HEN with uncertain or varying range of flowrate and temperature. The model is based on floating pinch concept. Two case studies are solved using the proposed model. It is proven that the model can handle situations with temperature-dependent heat capacity and varying operating parameters efficiently, and yet locates the rigorous hot and cold utility targets. The proposed model will be used to determine the hot and cold utility targets in the HIRCN that will be presented in following chapters.

CHAPTER 5: SYNTHESIS OF HIRCNs WITHOUT HEAT OF MIXING

5.1 Introduction

In this chapter, a generic methodology for the synthesis of heat integrated resource conservation networks (HIRCNs) without heat of mixing is presented. This methodology is established based on the general framework as presented in Chapter 3. Two case studies are solved to demonstrate the applicability of the developed methodology.

5.2 Problem statement

To formulate concentration- and property-based heat integrated resource conservation network (HIRCN) without heat of mixing, temperature constraints and heat exchanger network (HEN) are incorporated into concentration- and property-based resource conservation network (RCN). The problem to be addressed is given as follows:

Given *NSOURCES* number of process sources and *NSINKS* number of process sinks. Process sources may be allocated for reuse/recycle to the process sinks, or be discharge as waste. Each process source *i*, has a fixed flowrate (W_i), property operator ($\psi_{i,p}$) and temperature (T_i). Process sinks are units that can receive process sources. Each sink *j*, has an acceptable range of flowrate (G_j), property ($\psi_{j,p}$) and temperature (T_j), given as in Equations 5.1 – 5.3.

$$G_j^{\min} \le G_j \le G_j^{\max} \quad j \in NSINKS \tag{5.1}$$

$$\psi_{j,p}^{\min} \le \psi_{j,p} \le \psi_{j,p}^{\max} \quad j \in NSINKS \quad p \in NPROP \tag{5.2}$$

$$T_j^{\min} \le T_j \le T_j^{\max} \quad j \in NSINKS \tag{5.3}$$

where $G_j^{\min}$, $G_j^{\max}$, $\psi_{j,p}^{\min}$, $\psi_{j,p}^{\max}$, $T_j^{\min}$ and $T_j^{\max}$ are the respective lower and upper bounds of the admissible flowrate, property operator p and temperature for sink j. In addition, *NFRESH* number of external fresh resources are available at property operator p ($\psi_{r,p}$) and temperature (T_r) which may be supplemented to the sinks. The flowrate of fresh resource r is to be determined as part of the solution model.

A general linearised mixing rule is needed to define all possible mixing patterns among the individual properties, which can take the form of concentration, pH, density, etc. This can be given by Equation 5.4 that follows (Shelley and El-Halwagi, 2000):

$$\psi(\bar{p}) = \sum_m x_m \psi_{m,p} \tag{5.4}$$

where $\psi_{m,p}$ and $\psi(\bar{p})$ are the operators for property p of stream m and mixture property $\bar{p}$ respectively; while x_m is the fractional distribution of stream m of the total mixture flowrate.

In the HIRCN, a group of process streams is intended for the HEN. Note that these streams can take the form as a set of *NHOT* hot streams (that need cooling), or a set of *NCOLD* cold stream*s* (that need heating). The flowrates and inlet and outlet temperatures of these hot and cold streams need to be determined simultaneously within the HIRCN. Heat is to be recovered from hot streams to cold streams. Besides, external hot (Q_h) and cold (Q_c) utilities are available after maximising energy recovery between hot and cold streams. It is assumed that the compositions and flowrates of process streams remain unchanged after the HEN.

The overall objective is to synthesise a HIRCN of minimum cost, which may take the form of minimum annual operating cost (AOC) or total annualised cost (TAC).

5.3 Derivation of superstructure

The superstructure for the above-described problem is derived based on the general RCN representation and is given as a source-HEN-sink representation in Figure 5.1. As shown, each source is split and sent to all sinks; or being discharged as waste. Note that all streams will pass through the HEN.

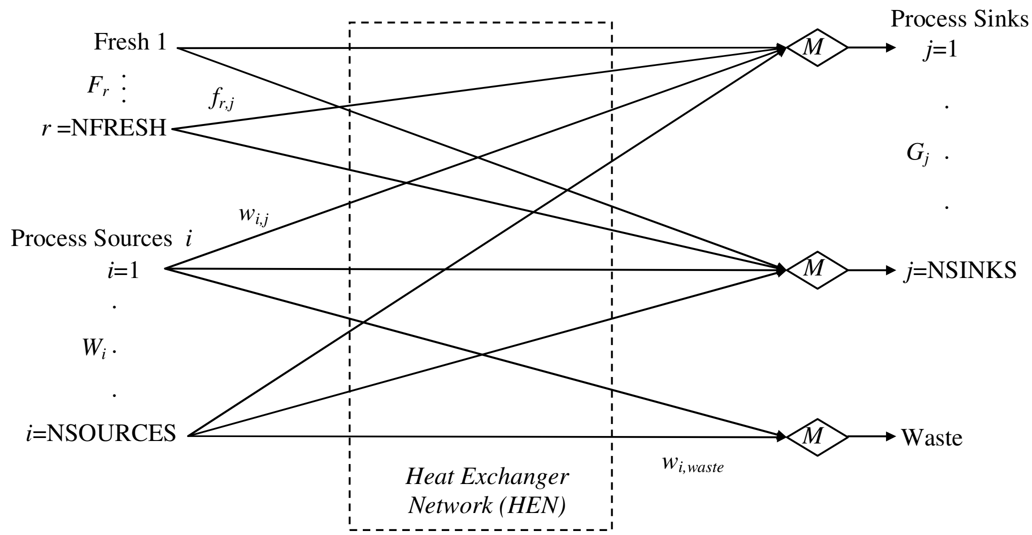


Figure 5.1: Source-HEN-sink representation for a HIRCN without heat of mixing based on general RCN representation.

To simplify the HEN formulation, advantages can be taken of the source and sink temperature limiting data. In this work, hot stream is defined as a stream with supply temperature (T_h^{in}) which is higher than target temperature (T_h^{out}); while cold stream has supply temperature (T_c^{in}) which is lower than target temperature (T_c^{out}). Therefore, based on the supply temperature of source i and the target temperature of sink j, each stream from source i to sink j ($w_{i,j}$) can be considered as either hot or cold stream. However, if source i temperature falls within the target temperature range of sink j, source i can be split into hot and cold streams. For instance, for a sink with acceptable temperature range of 300K – 400K, a source with temperature of 350K may be split into hot (T_h^{in} = 350K and T_h^{out} = 300K – 349K) and cold streams (T_c^{in} = 350K and T_c^{out} = 351K – 400K). In other words, the temperatures before

HEN and after HEN are set or bounded based on the source *i* and sink *j* temperatures respectively.

This simplification enables one to categorise the HEN streams as hot or/and cold streams and extract the respective temperatures directly from the given source and sink temperature limiting data. More importantly, it has significantly reduced the number of temperature variables and also the search space of this formulation.

5.4 Model formulation

The following sub-sections present the models for both concentration- and property-based RCN, as well as the HEN section of the HIRCN for cases without heat of mixing (refer to the source-HEN-sink superstructure in Figure 5.1).

Concentration- and property-based RCN

The mass and energy balances for various sources and sinks can be defined as follows:

Splitting of fresh resource *r*:

$$F_r = \sum_{j \in NSINKS} f_{r,j} \quad r \in NFRESH \tag{5.5}$$

where $f_{r,j}$ is the flowrate of fresh resource *r* to sink *j*.

Splitting of process source *i*:

$$W_i = \sum_{j \in NSINKS} w_{i,j} + B_{i,\text{waste}} \quad i \in NSOURCES \tag{5.6}$$

where $w_{i,j}$ and $B_{i,\text{waste}}$ are the flowrates of source *i* recovered to sink *j* and discharged as waste, respectively.

Mass balances at the mixing point before sink *j*:

$$G_j = \sum_{i \in NSOURCES} w_{i,j} + \sum_{r \in NFRESH} f_{r,j} \quad j \in NSINKS \tag{5.7}$$

where G_j is the total flowrate of sink *j*.

Mass balance of waste:

$$B^{\text{waste}} = \sum_{i \in NSOURCES} B_{i,\text{waste}} \tag{5.8}$$

where B^{waste} is the flowrate of waste.

Based on Equation 5.4, property balance for property *p* at the mixing point before sink *j*:

$$\psi_{j,p} G_j = \sum_{i \in NSOURCES} \left[\psi_{i,p} w_{i,j}\right] + \sum_{r \in NFRESH} \left[\psi_{r,p} f_{r,j}\right] \quad j \in NSINKS \quad p \in NPROP \tag{5.9}$$

Property balance at the mixing point before waste:

$$\psi_{\text{waste},p} B^{\text{waste}} = \sum_{i \in NSOURCES} \left[\psi_{i,p} B_{i,\text{waste}}\right] \quad p \in NPROP \tag{5.10}$$

where $\psi_{\text{waste},p}$ is the property operator *p* for waste.

Note that Equations 5.9 and 5.10 are used to determine the mean property value of each sink *j* and waste, respectively, and should be carried out for all concerned properties for each process sink.

As discussed previously, the same stream sent from fresh resource *r* and source *i* to sink *j* and waste can take the form as hot and cold streams, if its temperature falls in between the operating temperature range of the sink and waste. Therefore, Equations 5.11 - 5.13 are included in the model.

$$f_{r,j} = m^{\mathrm{H}}_{r,j} + m^{\mathrm{C}}_{r,j} \quad r \in NFRESH \qquad j \in NSINKS \tag{5.11}$$

$$w_{i,j} = m^{\mathrm{H}}_{i,j} + m^{\mathrm{C}}_{i,j} \quad i \in NSOURCES \qquad j \in NSINKS \tag{5.12}$$

$$B_{i,\mathrm{waste}} = m^{\mathrm{H}}_{i,\mathrm{waste}} + m^{\mathrm{C}}_{i,\mathrm{waste}} \quad i \in NSOURCES \tag{5.13}$$

where $m^{\mathrm{H}}_{r,j}$, $m^{\mathrm{H}}_{i,j}$, $m^{\mathrm{C}}_{r,j}$ and $m^{\mathrm{C}}_{i,j}$ are flowrates of hot and cold streams from fresh resource *r* and source *i* to sink *j*, respectively; $m^{\mathrm{H}}_{i,\mathrm{waste}}$ and $m^{\mathrm{C}}_{i,\mathrm{waste}}$ are the flowrate of hot and cold streams from source *i* to waste.

Energy balances at the mixing point before the sink *j*:

$$\begin{aligned} G_j CP_j (T_j - T_o) = & \sum_{r \in NFRESH} m^{\mathrm{H}}_{r,j} CP^{\mathrm{H}}_{r,j} (T^{\mathrm{H,out}}_{r,j} - T_o) + \sum_{r \in NFRESH} m^{\mathrm{C}}_{r,j} CP^{\mathrm{C}}_{r,j} (T^{\mathrm{C,out}}_{r,j} - T_o) \\ + & \sum_{i \in NSOURCES} m^{\mathrm{H}}_{i,j} CP^{\mathrm{C}}_{i,j} (T^{\mathrm{H,out}}_{i,j} - T_o) + \sum_{i \in NSOURCES} m^{\mathrm{C}}_{i,j} CP^{\mathrm{C}}_{i,j} (T^{\mathrm{C,out}}_{i,j} - T_o) \quad j \in NSINKS \end{aligned} \tag{5.14}$$

where CP_j, $CP^{\mathrm{H}}_{r,j}$, $CP^{\mathrm{H}}_{i,j}$, $CP^{\mathrm{C}}_{r,j}$, and $CP^{\mathrm{C}}_{i,j}$ are heat capacities of sink *j*, hot and cold streams from fresh resource *r* and source *i* to sink *j*, respectively; $T^{\mathrm{H,out}}_{r,j}$, $T^{\mathrm{H,out}}_{i,j}$, $T^{\mathrm{C,out}}_{r,j}$ and $T^{\mathrm{C,out}}_{i,j}$ are the target temperatures of hot and cold streams from fresh resource *r* and source *i* to sink *j*, respectively, while T_o is the reference temperature.

Energy balance at the mixing point before waste:

$$\begin{aligned} B^{\mathrm{waste}} CP^{\mathrm{waste}} (T^{\mathrm{waste}} - T_o) = & \sum_{i \in NSOURCES} m^{\mathrm{H}}_{i,\mathrm{waste}} CP^{\mathrm{H}}_{i,\mathrm{waste}} (T^{\mathrm{H,out}}_{i,\mathrm{waste}} - T_o) \\ + & \sum_{i \in NSOURCES} m^{\mathrm{C}}_{i,\mathrm{waste}} CP^{\mathrm{C}}_{i,\mathrm{waste}} (T^{\mathrm{C,out}}_{i,\mathrm{waste}} - T_o) \end{aligned} \tag{5.15}$$

where CP^{waste}, $CP^{\mathrm{H}}_{i,\mathrm{waste}}$ and $CP^{\mathrm{H}}_{i,\mathrm{waste}}$ are the heat capacities of waste, hot and cold streams from source *i* to waste, respectively; T^{waste}, $T^{\mathrm{H,out}}_{i,\mathrm{waste}}$ and $T^{\mathrm{C,out}}_{i,\mathrm{waste}}$ refer to the temperature of waste, target temperatures of hot and cold streams from source *i* to waste, respectively.

Heat exchanger network

The revised HEN floating pinch method established in Chapter 4 is applied in this model. As discussed in Section 4.3, the potential pinch candidates are those corner points on the composite curves which correspond to the inlet temperatures of any hot and cold streams (see Figure 4.1(a)). Therefore, overall energy balance equation and energy balance equation above or below pinch are developed for each of the postulated pinch point candidates, which will then identify the true pinch point and also the minimum hot and cold utilities. Detailed description of the revised HEN floating pinch method can be referred to Chapter 4. The following section presents the HEN model of the HIRCN without heat of mixing.

As stated in Chapter 4, the supply and target temperatures of the hot and cold streams from fresh resource r and source i to sink j and waste are first shifted based on minimum temperature of driving force, $\Delta T_{\min}$ (subtract $\Delta T_{\min}/2$ for hot streams; add $\Delta T_{\min}/2$ for cold streams). Based on the superstructure presented in Figure 5.1, Equations 4.7 – 4.10 are replaced by Equations 5.16 – 5.19 as follow,

$$T_h^{s} = \begin{bmatrix} T_{1,1}^{\text{in}} - \dfrac{\Delta T_{\min}}{2} \\ \vdots \\ T_{1,j}^{\text{in}} - \dfrac{\Delta T_{\min}}{2} \\ \vdots \\ T_{r,j}^{\text{in}} - \dfrac{\Delta T_{\min}}{2} \\ \vdots \\ T_{(r+i),j}^{\text{in}} - \dfrac{\Delta T_{\min}}{2} \\ T_{1,\text{waste}}^{\text{in}} - \dfrac{\Delta T_{\min}}{2} \\ \vdots \\ T_{i,\text{waste}}^{\text{in}} - \dfrac{\Delta T_{\min}}{2} \end{bmatrix} \quad \begin{array}{r} i \in NSOURCES \\ j \in NSINKS \\ r \in NFRESH \\ h \in NHOT \end{array} \tag{5.16}$$

$$T_h^{\mathrm{t}} = \begin{bmatrix} T_{1,1}^{\mathrm{out}} - \dfrac{\Delta T_{\min}}{2} \\ \vdots \\ T_{1,j}^{\mathrm{out}} - \dfrac{\Delta T_{\min}}{2} \\ \vdots \\ T_{r,j}^{\mathrm{out}} - \dfrac{\Delta T_{\min}}{2} \\ \vdots \\ T_{(r+i),j}^{\mathrm{out}} - \dfrac{\Delta T_{\min}}{2} \\ T_{1,\mathrm{waste}}^{\mathrm{out}} - \dfrac{\Delta T_{\min}}{2} \\ \vdots \\ T_{i,\mathrm{waste}}^{out} - \dfrac{\Delta T_{\min}}{2} \end{bmatrix} \quad \begin{matrix} i \in NSOURCES \\ j \in NSINKS \\ r \in NFRESH \\ h \in NHOT \end{matrix} \tag{5.17}$$

$$T_c^{\mathrm{s}} = \begin{bmatrix} T_{1,1}^{\mathrm{in}} - \dfrac{\Delta T_{\min}}{2} \\ \vdots \\ T_{1,j}^{\mathrm{in}} - \dfrac{\Delta T_{\min}}{2} \\ \vdots \\ T_{r,j}^{\mathrm{in}} - \dfrac{\Delta T_{\min}}{2} \\ \vdots \\ T_{(r+i),j}^{\mathrm{in}} - \dfrac{\Delta T_{\min}}{2} \\ T_{1,\mathrm{waste}}^{\mathrm{in}} - \dfrac{\Delta T_{\min}}{2} \\ \vdots \\ T_{i,\mathrm{waste}}^{\mathrm{in}} - \dfrac{\Delta T_{\min}}{2} \end{bmatrix} \quad \begin{matrix} i \in NSOURCES \\ j \in NSINKS \\ r \in NFRESH \\ c \in NCOLD \end{matrix} \tag{5.18}$$

$$T_c^{\mathrm{t}} = \begin{bmatrix} T_{1,1}^{\mathrm{out}} - \dfrac{\Delta T_{\min}}{2} \\ \vdots \\ T_{1,j}^{\mathrm{out}} - \dfrac{\Delta T_{\min}}{2} \\ \vdots \\ T_{r,j}^{\mathrm{out}} - \dfrac{\Delta T_{\min}}{2} \\ \vdots \\ T_{(r+i),j}^{\mathrm{out}} - \dfrac{\Delta T_{\min}}{2} \\ T_{1,\mathrm{waste}}^{\mathrm{out}} - \dfrac{\Delta T_{\min}}{2} \\ \vdots \\ T_{i,\mathrm{waste}}^{out} - \dfrac{\Delta T_{\min}}{2} \end{bmatrix} \qquad \begin{array}{c} i \in NSOURCES \\ j \in NSINKS \\ r \in NFRESH \\ c \in NCOLD \end{array} \tag{5.19}$$

where T_h^{s} and T_h^{t} are shifted supply and target temperatures of the hot stream, while T_c^{s} and T_c^{t} are shifted supply and target temperatures of the cold streams in HEN. Note that the size of *NHOT* and *NCOLD* set is $j(r+i)+i$ respectively.

The potential pinch candidate, T_q are taken as the inlet temperatures of the hot and cold streams (refer to Equation 4.11). To identify the true pinch point and the minimum hot and cold utilities, the total energy balance (Equation 4.30) is solve together with either energy balance above the pinch point candidates (Equation 4.20) with the respective constraints (Equations 4.16 - 4.19) or energy balance below the pinch point candidates (Equation 4.29) with the respective constraints (Equations 4.25 − 4.28).

In order to ensure the connection between concentration- and property-based RCN model and HEN model, Equations 5.20 – 5.26 are used to relate the flowrates and temperatures in these models.

Flowrate of hot and cold streams from fresh resource *r* and source *i* to sink *j* are classified as follow,

$$m_h = \begin{bmatrix} m_{1,1}^{\mathrm{H}} \\ \vdots \\ m_{1,j}^{\mathrm{H}} \\ \vdots \\ m_{r,j}^{\mathrm{H}} \\ \vdots \\ m_{(r+i),j}^{\mathrm{H}} \\ m_{1,\mathrm{waste}}^{\mathrm{H}} \\ \vdots \\ m_{i,\mathrm{waste}}^{\mathrm{H}} \end{bmatrix} \quad \begin{matrix} i \in NSOURCES \\ j \in NSINKS \\ r \in NFRESH \\ h \in NHOT \end{matrix} \tag{5.20}$$

$$m_c = \begin{bmatrix} m_{1,1}^{\mathrm{C}} \\ \vdots \\ m_{1,j}^{\mathrm{C}} \\ \vdots \\ m_{r,j}^{\mathrm{C}} \\ \vdots \\ m_{(r+i),j}^{\mathrm{C}} \\ m_{1,\mathrm{waste}}^{\mathrm{C}} \\ \vdots \\ m_{i,\mathrm{waste}}^{\mathrm{C}} \end{bmatrix} \quad \begin{matrix} i \in NSOURCES \\ j \in NSINKS \\ r \in NFRESH \\ c \in NCOLD \end{matrix} \tag{5.21}$$

Supply temperature of hot and cold streams from fresh resource *r* and source *i* to sink *j* are the same as that of fresh resource *r* and source *i*.

$$T_{r,j}^{\mathrm{H,in}} = T_{r,j}^{\mathrm{C,in}} = T_r \quad r \in NFRESH \quad j \in NSINKS \tag{5.22}$$

$$T_{i,j}^{\mathrm{H,in}} = T_{i,j}^{\mathrm{C,in}} = T_i \quad i \in NSOURCES \quad j \in NSINKS \tag{5.23}$$

Target temperature of hot and cold streams from fresh resource *r* and source *i* to sink *j* are based on the temperature of sink *j*.

$$T_{r,j}^{\mathrm{H,\,out}} = T_{r,j}^{\mathrm{C,\,out}} = T_j \quad r \in NFRESH \quad j \in NSINKS \tag{5.24}$$

$$T_{i,j}^{\mathrm{H,\,out}} = T_{i,j}^{\mathrm{C,\,out}} = T_j \quad i \in NSOURCES \qquad j \in NSINKS \tag{5.25}$$

Supply and target temperatures of hot and cold streams from source *i* to waste are the same as those of source *i* and waste.

$$T_{i,\mathrm{waste}}^{\mathrm{H,\,in}} = T_{i,\mathrm{waste}}^{\mathrm{C,\,in}} = T_i \quad i \in NSOURCES \tag{5.26}$$

$$T_{i,\mathrm{waste}}^{\mathrm{H,\,out}} = T_{i,\mathrm{waste}}^{\mathrm{C,\,out}} = T^{\mathrm{waste}} \quad i \in NSOURCES \tag{5.27}$$

5.5 Solution strategy

It is worth noting that the superstructure derived (Figure 5.1) is a generic HIRCN representative, where each source is split and directly supplied to all sinks or be discharged as waste, and all these streams are involved in the HEN. Besides, the proposed model is an MINLP model as the supply and target temperatures as well as the property operator *p* for each hot stream *h* and cold stream *c* (T_h^{in}, T_h^{out}, T_c^{in}, T_c^{out}, $\psi_{h,p}$ and $\psi_{c,p}$) in Equations 4.20, 4.29, 4.30, and 5.9 are unknown variables. However, the problem formulation enables the supply and target temperatures of the hot and cold streams in HEN to be known values or range as they are directly based on the temperature of sources and sinks. As a result, the proposed model is convex and can be solved easily using software such as LINGO. Thus, a specific solution strategy is not required for this problem as the solver is able to provide the global optimal solution. Note that the solution obtained consists of the minimum cost of a HIRCN, which may take the form of AOC or TAC. The optimal solution also includes the flowrate of fresh resources *r*, external hot and cold utilities, as well as the flowrates of all process streams in the source-HEN-sink superstructure.

5.6 Network configuration

In order to achieve a complete a HIRCN configuration, one needs to have the RCN structure as well as the HEN design for a given problem. The RCN result can be obtained directly from the optimal solution of the proposed model. However, for HEN, only the external hot and cold utilities are determined as a result of the optimisation problem (i.e. without any HEN design). Therefore, the HEN is synthesised using the classical *pinch design method* (Linnhoff and Flower, 1978a; Linnhoff et al., 1982; Smith, 2005). This additional step also serves as a verification of the hot and cold utility targets obtained in the optimisation approach.

5.7 Case studies

To illustrate the proposed model, Case studies 1 and 2 presented in Chapter 3 are solved using Extended LINGO v13.0 with Global Solver in a computer with a Core i3, 3.3 GHz processor. In these case studies, total operating hour (k) is taken as 8000 h/y.

5.7.1 Case study 1

Case study 1 is an ammonia recovery case study taken from Sahu and Bandyopadhyay (2012). The limiting data for this case study is showed in Table 3.1. In addition, it is given that the available fresh ammonia is supplied at 30^{o}C, with unit cost of \$500/ton (Cost$_r$) and waste ammonia has to be discharged at 40^{o}C (Sahu and Bandyopadhyay, 2012). In this case study, the costs of hot and cold utilities (Cost$_h$ and Cost$_c$) are given as 3.758 \$/kW.h and 0.005 \$/kW.h respectively. Moreover, the major component in all stream is ammonia; thus, heat capacities of all streams (CP_i , CP_j , CP_r , $CP_{r,j}^{\mathrm{H}}$, $CP_{i,j}^{\mathrm{H}}$, $CP_{r,j}^{\mathrm{C}}$, $CP_{i,j}^{\mathrm{C}}$ CP^{waste} , $CP_{i,\mathrm{waste}}^{\mathrm{H}}$ and $CP_{i,\mathrm{waste}}^{\mathrm{C}}$) are assumed to take a constant value of 2.19 kJ/kg.K; and $\Delta T_{\min}$ of 35^{o}C is used (Sahu and Bandyopadhyay, 2012).

The objective of this case study is to minimise AOC, which consists of operating costs for fresh resources, as well as hot and cold utilities in the HIRCN. The optimisation objective is formulated as follows:

$$\min_{F_r, Q_h, Q_c} AOC = k * \left\{ \sum_{r=1}^{NFRESH} \text{Cost}_r F_r + \text{Cost}_h Q_h + \text{Cost}_c Q_c \right\} \tag{5.28}$$

where Cost_r is the cost of fresh resources.

Equation 5.28 is solved subject to the constraints in Equations 4.11, 4.16 – 4.20, 4.30 and 5.5 – 5.27. The objective value of \$ 9.44 x 10^9 /yr is obtained in 3 CPU seconds. The optimised HIRCN is showed in Figure 5.2. As shown, the HIRCN consume a fresh water flowrate (F_r) of 654.9 kg/s, and with utility targets of Q_h = 132,927 kW and Q_c = 79,228 kW as well as true pinch point of 112.5ºC. Meanwhile, the HEN design for this case study is shown in Figure 5.3, which shows the same energy targets as the proposed model. The LINGO code and solution for this case study can be found in Appendix C.

Note that in this case study, the unit cost of fresh ammonia is much higher than that of hot and cold utilities. As a result, fresh ammonia is minimised while higher consumption of utilities is experienced. It is worth mentioning that the results are identical with the reported results in the original work (Sahu and Bandyopadhyay, 2012), if a two stage LP model is solved such as that in Case study 1.

5.7.2 Case study 2

Case study 2 is adapted from Nápoles-Rivera et al. (2010), where multiple properties are considered. Table 3.2 shows the limiting data for process sinks and sources for this case study.

Equations 5.29 – 5.32 outline the mixing rules for toxicity (*Tox*), theoretical oxygen demand (*THOD*), density (ρ) and viscosity (μ) (Nápoles-Rivera et al., 2010),

$$\overline{Tox} = \sum_m x_m Tox_m \tag{5.29}$$

$$\overline{THOD} = \sum_m x_m THOD_m \tag{5.30}$$

$$\overline{\rho} = \sum_m x_m \frac{1}{\rho_m} \tag{5.31}$$

$$\overline{\mu} = \sum_m x_m \log \mu_m \tag{5.32}$$

In addition, mixing rules of pH for different pH range (Hortua et al., 2012) are also given as follow.

For acid mixing ($0 \le pH \le 7$):

$$\overline{10^{-pH}} = \sum_m x_m 10^{-pH_m} \tag{5.33}$$

For base mixing ($7 \le pH \le 14$):

$$\overline{10^{pH-14}} = \sum_m x_m 10^{pH_m-14} \tag{5.34}$$

For neutralisation between acid and base streams, it is given by:

$$10^{-pH} = \sum_{Acid} x_{acid} 10^{-pH_{acid}} - \sum_{Base} x_{base} 10^{-pH_{base}} \tag{5.35}$$

Unit cost for fresh resource (Cost$_r$) (Nápoles-Rivera et al., 2010), hot and cold utilities (Cost$_h$ and Cost$_c$) are given as 0.0009 \$/lb, 0.000659 \$/Btu and 0.0000015 \$/Btu respectively. In addition, $\Delta T_{\min}$ of 10°C is used. As the process streams in this case study are mainly water, heat capacities of all streams (CP_i, CP_j, CP_r, $CP^{\mathrm{H}}_{r,j}$, $CP^{\mathrm{H}}_{i,j}$, $CP^{\mathrm{C}}_{r,j}$, $CP^{\mathrm{C}}_{i,j}$ CP^{waste}, $CP^{\mathrm{H}}_{i,\mathrm{waste}}$ and $CP^{\mathrm{C}}_{i,\mathrm{waste}}$) are assumed to be a constant value of 1.8 Btu/lb°C.

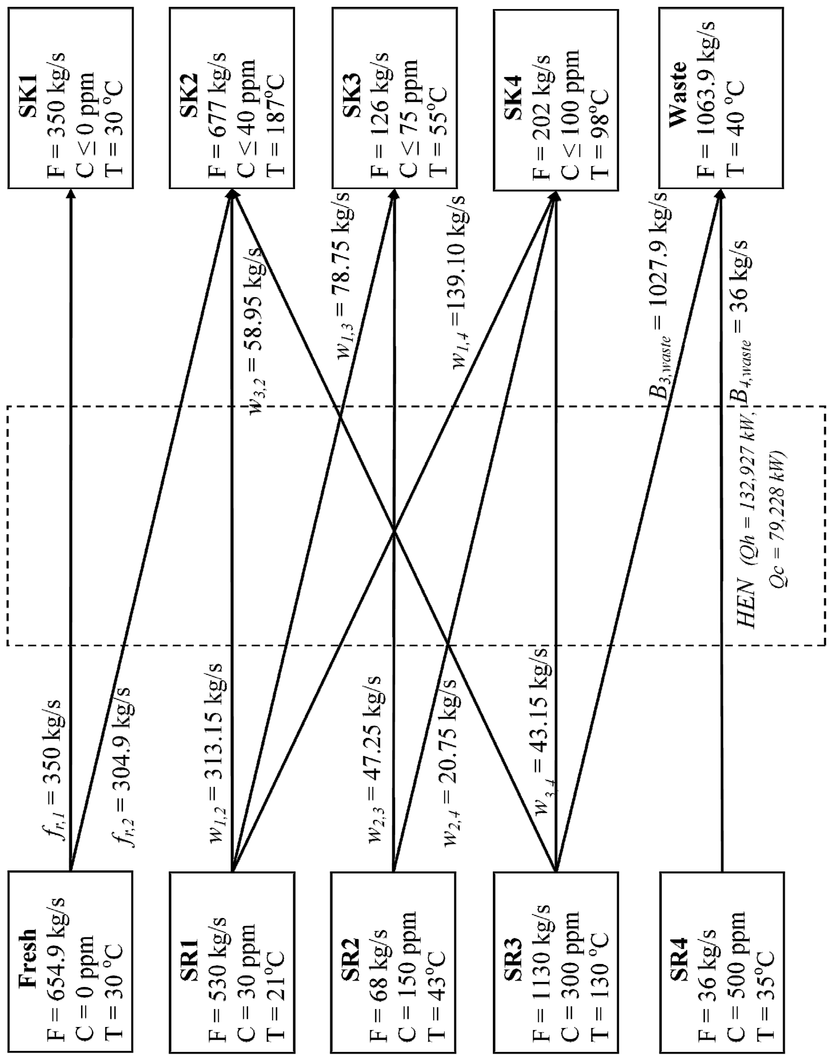


Figure 5.2: Optimal HIRCN solution for Case study 1.

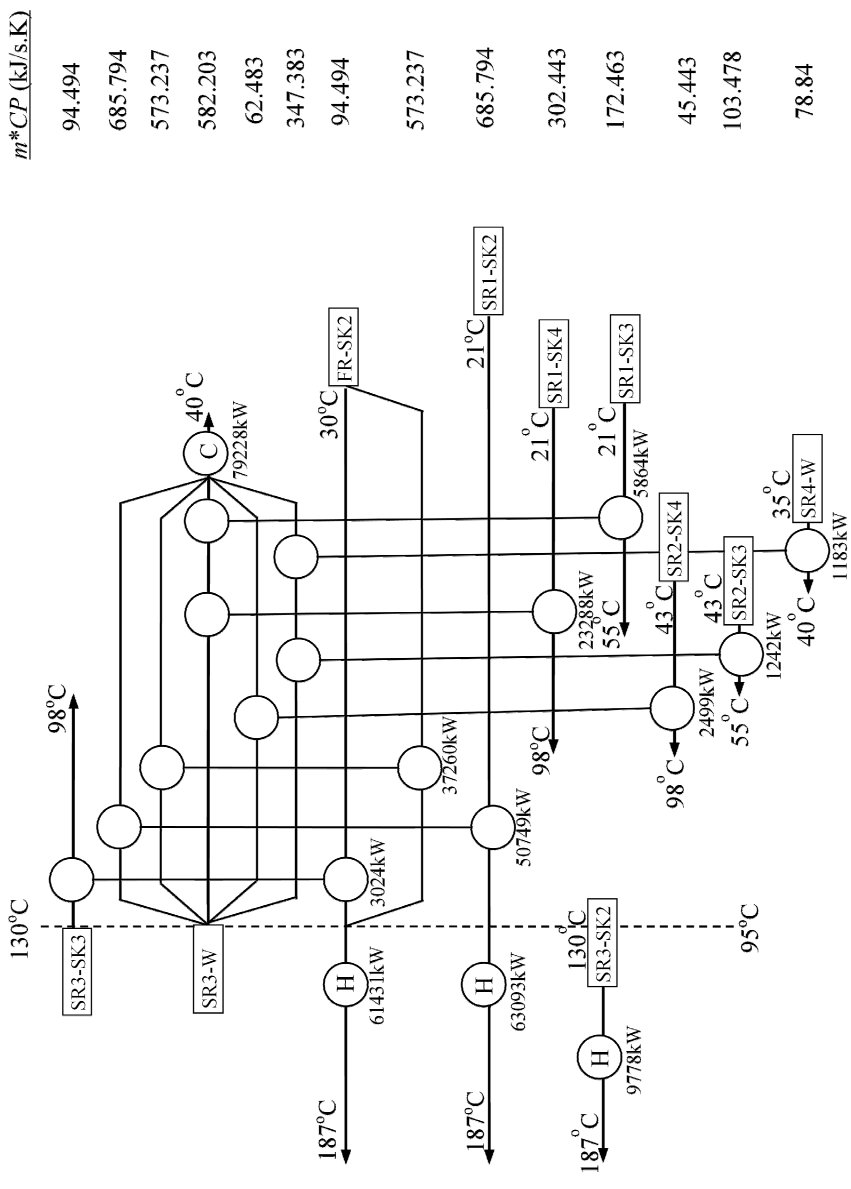


Figure 5.3: HEN for Case study 1.

The objective of this case study is to minimise annual operating cost (AOC), which consists of operating costs for fresh resources, as well as hot and cold utilities in the HIRCN. Solving the optimisation objective in Equation 5.28, subject to the constraints in Equations 4.11, 4.17 – 4.22, 5.1 – 5.3, 5.5 – 5.27 and 5.29 – 5.35 yields the minimum AOC of $ 254,631, with the optimal values of F_r, Q_h and Q_c determined as 3,523 lb/h, 0 Btu/h and 80,786 Btu/h, respectively. The optimal HIRCN and the HEN design for this case study are shown in Figure 5.4 and Figure 5.5. Note that the energy targets are identical as per that obtained via the proposed model. Note that the LINGO code and solution for this case study can be found in Appendix D.

Additionally, Case study 2 is also solved via a two-stage optimisation approach (Foo, 2012) for comparison with the proposed approach. In the first stage, the optimisation objective is set to minimise the fresh water flowrate as follow,

$$\text{Minimise } F_r \tag{5.36}$$

Equation 5.36 is solved subject to the constraints in Equations 5.1 – 5.2 and 5.5 – 5.10; which yields F_r of 3,523 lb/h. This is then added as a new constraint to the problem in the second stage, i.e.,

$$F_r = 3{,}523 \tag{5.37}$$

The optimisation objective in the second stage is set to minimise hot utility:

$$\text{Minimise } Q_h{*}\text{Cost}_h + Q_c{*}\text{Cost}_c \tag{5.38}$$

Solving Equation 5.38 subject to constraints in Equation 4.11, 4.25 – 4.30, 5.1 – 5.3, 5.5 – 5.27, 5.29 – 5.35 and 5.37 yield minimum Q_h and Q_c of 0 Btu and 80,786 Btu, respectively in 5 CPU seconds. This shows the same results as the proposed model. This is mainly due to the higher fresh resources cost as compared to the hot and cold utilities cost in this case study. Thus, when the case study is solved using the proposed simultaneous approach F_r is first minimised followed by Q_h and Q_c. Note that for cases with fresh resources cost that is compatible with hot and cold utilities cost, the results from the proposed simultaneous approach will not be the same as those from sequential approach. In these situations, the proposed simultaneous approach will choose to minimise fresh resources as well as hot and cold utilities simultaneously.

5.8 Chapter summary

A new generic methodology for the synthesis of HIRCNs without heat of mixing is presented in this chapter. An MINLP formulation has been developed to identify the minimum cost of a HIRCN, which simultaneously optimised the fresh resources as well as the external hot and cold utilities. Furthermore, the model is able to solve for problems with varied process parameters (e.g. flowrates, temperatures and properties). Two case studies are used to demonstrate the proposed methodology.

However, the main limitation of the methodology is that, the model is not applicable for situations where heat of mixing is involved. The is because heat of mixing results in energy generation (exothermic mixing) or absorption (endothermic mixing) of the mixture at the inlet of each sink (due to mixing of various $w_{i,j}$), which then increases/decreases the temperature of the mixture. For cases where sinks have fixed temperatures, the mixture temperature may be higher or lower than its limiting temperature. Thus, the sink temperature constraint will not be fulfilled; which leads to infeasible solution. In another case, even though the temperature constraint may be fulfilled (if the energy produced or consumed by heat of mixing is insignificant), there is still a high possibility that the temperature constraints may be violated. As a result of this limitation, another superstructure is presented in Chapter 6 for cases that encounter the effect of heat of mixing.

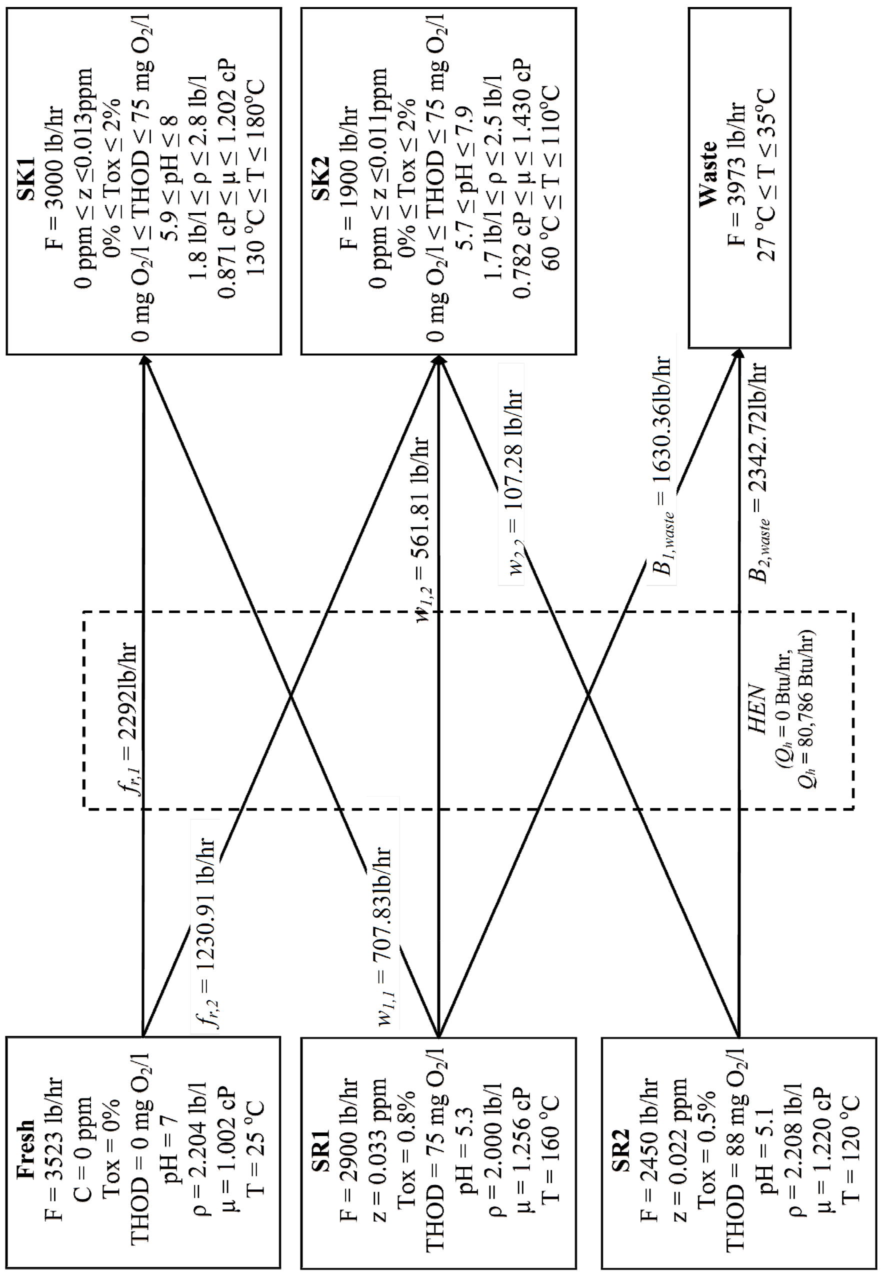


Figure 5.4: : Optimal HIRCN solution for Case study 2

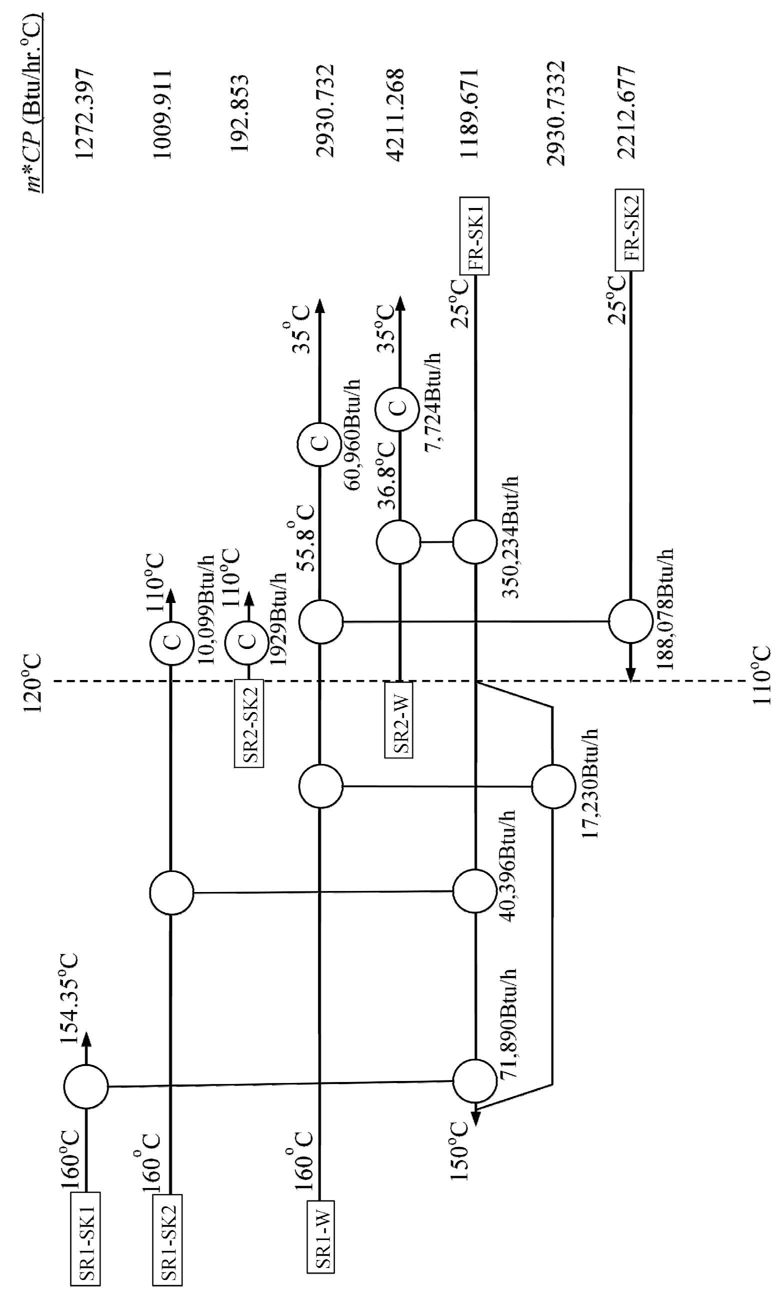


Figure 5.5: HEN for Case study 2.

CHAPTER 6: SYNTHESIS OF HIRCNs WITH HEAT OF MIXING

6.1 Introduction

When two or more process streams are mixed together, heat of mixing occurs and causes temperature changes in a system. Nevertheless, the model for HIRCN synthesis in Chapter 5 does not consider cases that involve heat of mixing. Thus, a generic model for the synthesis of HIRCNs that considers heat of mixing is presented in this chapter. This methodology is also developed based on the general framework for HIRCNs as illustrated in Chapter 3. To demonstrate the applicability of the developed methodology, two case studies are solved at the end of this chapter.

6.2 Problem statement

The problem definition of a HIRCN with heat of mixing is given as follows:

Given *NSOURCES* number of process sources that can be considered for reuse/recycle in the process sinks, or be discharged as waste. Given also *NSINKS* number of process sinks which are units that can accept process sources. Each process source i, has fixed flowrate (W_i), property operator p ($\psi_{i,p}$) and temperature (T_i). Each sink j, has an acceptable range of flowrate (G_j), property operator p ($\psi_{j,p}$) and temperature (T_j), given as in Equations 5.1 – 5.3. *NFRESH* number of external fresh resources may be purchased to supplement the requirement of the sinks. Each fresh resource r has property operator p ($\psi_{r,p}$) and temperature (T_r); and its flowrate is to be determined as part of the solution model. Furthermore, a general linearised mixing rule as given in Equation 5.4 is needed to identify all possible mixing patterns for each property.

The HIRCNs with heat of mixing problem can be represented by a source-HEN-sink superstructure given as in Figure 6.1. Each source is segregated and supplied to all sinks directly. Besides, each source is also split and be sent to all mixing points before the heat exchanger network (HEN). These mixed streams are classified into a set of *NHOT* hot streams and a set of *NCOLD* cold streams for the HEN. Hot stream is defined as a stream with supply temperature higher (T_h^{in}) than the target temperature (T_h^{out}); while cold stream has supply temperature (T_c^{in}) lower than the target temperature (T_c^{out}). The flowrates as well as inlet and outlet temperatures of the hot and cold streams are to be determined as part of the solution of the HIRCN model. Heat is to be recovered from the hot streams to cold streams. Besides, external hot (Q_h) and cold (Q_c) utilities are available after maximising energy recovery between the hot and cold streams. After HEN, these streams are then segregated at the splitting points to be sent to all sinks. Heat of mixing occurs at both the mixing points before HEN and those before process sinks.

The objective of this work is to synthesise a HIRCN with minimum cost, which may take the form of minimum annual operating cost (AOC) or total annualised cost (TAC).

6.3 Derivation of superstructure

Heat of mixing plays an important role in representing how systems of gases or liquids undergo temperature change as a result of mixing of process streams. However, the superstructure presented in Chapter 5 is unable to handle HIRCNs with heat of mixing. Therefore, a new superstructure with the consideration of heat of mixing is proposed in Figure 6.1.

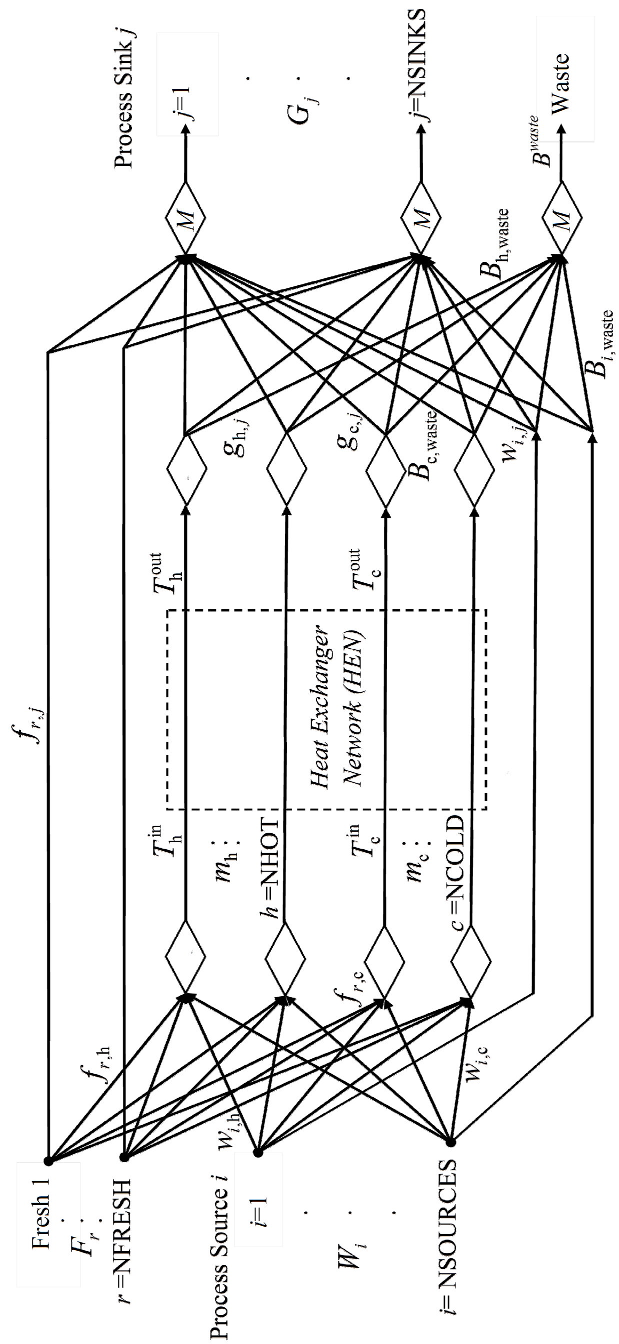


Figure 6.1: Source-HEN-sink representation for a HIRCN with heat of mixing.

For the superstructure shown in Figure 6.1, the supply and target temperatures of the HEN are not fixed using the limiting data of the process sinks and sources (such as those in the superstructure in Chapter 5). Instead, the supply temperature is calculated using an energy balance equation (with heat of mixing) based on the flowrates of process sources and fresh resources; while the target temperature can take any value that fulfills the temperature constraints of the process sink. Note that in this case, the flowrates of process sources and fresh resources, as well as the target temperature of the hot and cold streams in the HEN are to be determined as part of the solution model.

This superstructure is derived in such a way that it includes all possibilities on stream mixing before HEN, stream splitting after HEN, stream mixing before each sink and sources bypassing the HEN. These possibilities are important to ensure that opportunities for heat of mixing are included as it may affect the results of HEN which will directly impact on the solution of the problem formulation. Note that this is a unique and a newly presented superstructure found in the open literature. Furthermore, this superstructure is robust as it can be viewed as generic model that embeds various configurations. For instance, when $w_{i,j}$ and $f_{r,j}$ are set to be zero, and $g_{h,j}$ and $g_{h,j}$ are only allowed for the respective sink j, the superstructure becomes a sub-superstructure (Figure 6.2) which only consists of splitting of source i to mixing points before entering HEN, and the split sources are sent directly to its respective sinks after the HEN.

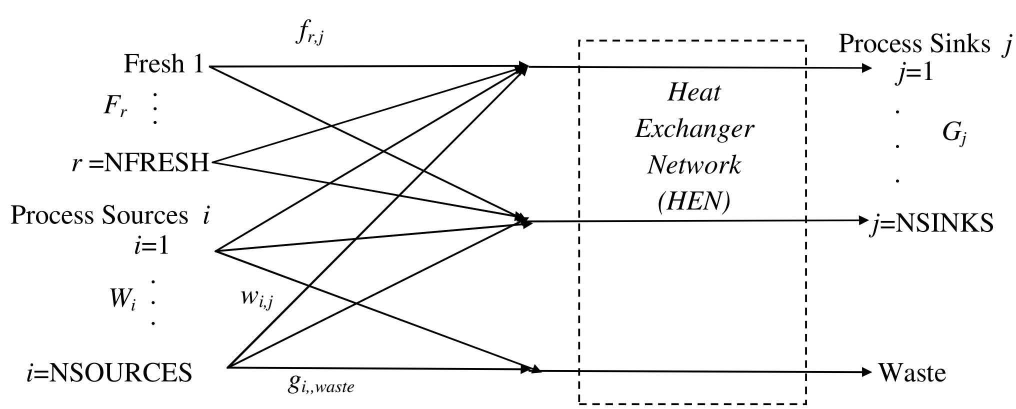


Figure 6.2: Sub-superstructure of HIRCN with heat of mixing.

6.4 Model formulation

In the following section, both models for concentration- and property-based RCN as well as HEN of the HIRCN with heat of mixing are presented.

Concentration- and property-based RCN

For each node of the HIRCN with heat of mixing in Figure 6.1, its mass and energy balances can be defined as follows:

Splitting of fresh resource *r*:

$$F_r = \sum_{j \in NSINKS} f_{r,j} + \sum_{h \in NHOT} f_{r,h} + \sum_{c \in NCOLD} f_{r,c} \quad r \in NFRESH \tag{6.1}$$

where $f_{r,j}$, $f_{r,h}$ and $f_{r,c}$ are the flowrates of fresh resource *r* to sink *j* as well as to hot stream *h* and cold stream *c* in HEN respectively.

Splitting of process source *i*:

$$W_i = \sum_{j \in NSINKS} w_{i,j} + \sum_{h \in NHOT} w_{i,h} + \sum_{c \in NCOLD} w_{i,c} + B_{i,waste} \quad i \in NSOURCES \tag{6.2}$$

where $w_{i,j}$, $w_{i,h}$, $w_{i,c}$ and $B_{i,waste}$ are the flowrates of source *i* recovered to sink *j*, to hot stream *h* and cold stream *c* in HEN and to be discharged as waste, respectively.

Mass balances of hot stream *h* and cold stream *c* at the mixing point before HEN are

$$m_h = \sum_{i \in NSOURCES} w_{i,h} + \sum_{r \in NFRESH} f_{r,h} \quad h \in NHOT \tag{6.3}$$

$$m_c = \sum_{i \in NSOURCES} w_{i,c} + \sum_{r \in NFRESH} f_{r,c} \quad c \in NCOLD \tag{6.4}$$

where m_h and m_c are the flowrates of hot stream *h* and cold stream *c*.

Based on Equations 6.3 and 6.4, property balances for property *p* of hot stream *h* and cold stream *c* at the mixing point before HEN are

$$\psi_{h,p} m_h = \sum_{i \in NSOURCES} \left[\psi_{i,p} w_{i,h} \right] + \sum_{r \in NFRESH} \left[\psi_{r,p} f_{r,h} \right] \; h \in NHOT \quad p \in NPROP \tag{6.5}$$

$$\psi_{c,p} m_c = \sum_{i \in NSOURCES} \left[\psi_{i,p} w_{i,c} \right] + \sum_{r \in NFRESH} \left[\psi_{r,p} f_{r,c} \right] \; c \in NCOLD \quad p \in NPROP \tag{6.6}$$

where $\psi_{i,p}$, $\psi_{r,p}$, $\psi_{h,p}$ and $\psi_{c,p}$ are the property operator *p* for source *i*, fresh resource *r*, hot stream *h* and cold stream *c* in HEN, respectively.

As heat of mixing is taken into consideration, the energy balances of hot stream *h* and cold stream *c* at the mixing point before HEN are

$$m_h CP_h (T_h^{\text{in}} - T_o) = \sum_{i \in NSOURCES} w_{i,h} CP_i (T_i - T_o) + \sum_{r \in NFRESH} f_{r,h} CP_r (T_r - T_o) + m_h \Delta H_h^{\text{mix}} \quad h \in NHOT \tag{6.7}$$

$$m_c CP_c (T_c^{\text{in}} - T_o) = \sum_{i \in NSOURCES} w_{i,c} CP_i (T_i - T_o) + \sum_{r \in NFRESH} f_{r,c} CP_r (T_r - T_o) + m_c \Delta H_c^{\text{mix}} \quad c \in NCOLD \tag{6.8}$$

where CP_h, CP_c, CP_i, CP_r are the heat capacities of source *i*, fresh resource *r*, hot stream *h* and cold stream *c* respectively; T_o, T_i and T_r are the reference temperature and the temperatures of source *i* and fresh resource *r* while ΔH_h^{mix} and ΔH_c^{mix} are heat of mixing of hot and cold streams respectively.

Mass balance of hot stream *h* and cold stream *c* at the splitting point after HEN is

$$m_h = \sum_{j \in NSINKS} g_{h,j} + B_{h,\text{waste}} \quad h \in NHOT \tag{6.9}$$

$$m_c = \sum_{j \in NSINKS} g_{c,j} + B_{c,\text{waste}} \quad c \in NCOLD \tag{6.10}$$

where $g_{h,j}$ and $g_{c,j}$ are the flowrates of hot stream h and cold stream c in HEN to sink j, while $B_{h,\text{waste}}$ and $B_{c,\text{waste}}$ are the flowrates of hot stream h and cold stream c in HEN to be discharged as waste, respectively.

Mass balances at the mixing point before sink j:

$$G_j = \sum_{i \in NSOURCES} w_{i,j} + \sum_{r \in NFRESH} f_{r,j} + \sum_{h \in NHOT} g_{h,j} + \sum_{c \in NCOLD} g_{c,j} \quad j \in NSINKS \tag{6.11}$$

where G_j is the total flowrate of sink j.

Mass balance of waste:

$$B^{\text{waste}} = \sum_{i \in NSOURCES} B_{i,\text{waste}} + \sum_{h \in NHOT} B_{h,\text{waste}} + \sum_{c \in NCOLD} B_{c,\text{waste}} \tag{6.12}$$

where B^{waste} is the flowrate of waste.

Property balance for property p at the mixing point before sink j:

$$\psi_{j,p} G_j = \sum_{i \in NSOURCES} \left[\psi_{i,p} w_{i,j}\right] + \sum_{r \in NFRESH} \left[\psi_{r,p} f_{r,j}\right] + \sum_{c \in NHOT} \left[\psi_{h,p} g_{h,j}\right] + \sum_{c \in NCOLD} \left[\psi_{c,p} g_{c,j}\right]$$
$$j \in NSINKS \quad p \in NPROP \tag{6.13}$$

Note that Equations 6.5, 6.6 and 6.13 are used to determine the mean property value of each hot stream h, cold stream c and sink j, and should be carried out for all properties in concern for each hot stream, cold stream and process sink.

Energy balances involving heat of mixing at the mixing point before sink j:

$$G_j CP_j (T_j - T_o) = \sum_{i \in NSOURCES} w_{i,j} CP_i (T - T_o)_i + \sum_{r \in NFRESH} f_{r,j} CP_r (T_r - T_o) + \sum_{h \in NHOT} g_{h,j} CP_h (T_h^{\text{out}} - T_o)$$
$$+ \sum_{c \in NCOLD} g_{c,j} CP_c (T_c^{\text{out}} - T_o) + F_j \Delta H_j^{\text{mix}} \quad j \in NSINKS \tag{6.14}$$

where CP_j, T_j and ΔH_j^{mix} s the heat capacity of sink j, the temperature of sink j and the heat of mixing of sink j, respectively.

Energy balance at the mixing point before waste:

$$B^{\text{waste}} CP^{\text{waste}} (T^{\text{waste}} - T_o) = \sum_{i \in NSOURCES} B_{i,\text{waste}} CP_i (T_i - T_o) + \sum_{h \in NHOT} B_{h,\text{waste}} CP_h (T_h^{\text{out}} - T_o)$$
$$+ \sum_{c \in NCOLD} B_{c,\text{waste}} CP_c \ (T_c^{\text{out}} - T_o) + B^{\text{waste}} \Delta H_{\text{waste}}^{\text{mix}} \tag{6.15}$$

where CP^{waste}, T^{waste} and $\Delta H_{\text{waste}}^{\text{mix}}$ are the heat capacity, temperature and heat of mixing of waste discharge, respectively.

The generic term for heat of mixing used in Equations 6.7, 6.8, 6.14 and 6.15 can be determined as (Perry and Green, 1997),

$$\Delta H^{\text{mix}} = -RT^2 \left[\frac{\partial \left(\frac{G^E}{RT} \right)}{\partial T} \right]_{P,x} \tag{6.16}$$

where G^E, T, P and x are the excess Gibbs free energy, the absolute temperature, pressure and mole fraction respectively; while R is the ideal gas constant (8.314J/K mol). The excess Gibbs free energy can be estimated via various model such as Wilson, NRTL, Margules and van Laar equations (Perry and Green, 1997). Note that the excess Gibbs free energy is the difference between the actual value of Gibbs free energy for real solution and that of the ideal mixture, evaluated at the same composition, temperature and pressure.

Heat exchanger network

Owing to the varying flowrates and temperatures in the problem formulation, the revised HEN floating pinch method presented in Chapter 4 is used. The following section presents the HEN model of the HIRCNs with heat of mixing.

The supply and target temperatures of the hot and cold streams are first shifted by subtracting $\Delta T_{\min}/2$ for hot streams; while adding $\Delta T_{\min}/2$ for cold streams. These temperatures are given by Equations 4.7 – 4.10. The inlet temperatures of the hot and cold streams are taken as the potential pinch candidate, T_q (as shown in Equation 4.11). To identify the true pinch point and to ensure thermodynamic feasibility, the total energy balance (Equation 4.22) is to be used together with energy balance above the pinch point candidate (Equation 4.16) with the respective constraints (Equations 4.12 - 4.15). Alternatively, one may also make use of the energy balance below the pinch point candidate (Equation 4.21) with its respective constraints (Equations 4.17 - 4.20).

6.5 Solution strategy

As shown in Equations 4.16, 4.21, 4.22, 6,5, 6.6 and 6.13 the supply and target temperatures, as well as the property operator p for each hot stream h and cold stream c (T_h^{in}, T_h^{out}, T_c^{in}, T_c^{out}, $\psi_{h,p}$ and $\psi_{c,p}$) are unknown variables; this leads to a MINLP model. As the proposed model results in large and highly complex model in both nonlinearity and integer aspects, it is computational expensive. Furthermore, when the MINLP model is solved using Extended LINGO v13.0 with Global Solver, no solution is achieved due to non-convergence. In order to overcome this issue, the *discretisation approach* presented by Pham et al. (2009) is adopted in this work. According to Pham et al. (2009) the unknown variables are discretised into several known values. As a result of this, it transforms the formulation into MILP model which enable global optimum solution to be obtained. With sufficient discretisation, the global solution of the discretised problem can approximate (or coincide with) the true global optimal of the original problem (Pham et al., 2009). The following section explains the proposed strategy in detail.

Step 1: Discretisation of property operators for each hot and cold stream

In this thesis, the use of property operators $\psi_{h,p}$ and $\psi_{c,p}$ is taken as the discretised variables. The property operators of hot stream h and cold stream c are bounded by the property operators of the fresh resources, process sources and process sinks.

Using the following notation: $\psi_{HEN,p}^{\min} = \min\{\psi_{r,p},\ \psi_{i,p},\ \psi_{j,p}\}$ and $\psi_{HEN,p}^{\max} = \max\{\psi_{r,p},\ \psi_{i,p},\ \psi_{j,p}\}$, then the domain of $\psi_{h,p}$ and $\psi_{c,p}$ are given as follow,

$$\psi_{HEN,p}^{\min} \le \psi_{h,p} \le \psi_{HEN,p}^{\max} \tag{6.17}$$

$$\psi_{HEN,p}^{\min} \le \psi_{c,p} \le \psi_{HEN,p}^{\max} \tag{6.18}$$

where $\psi_{HEN,p}^{\min}$ and $\psi_{HEN,p}^{\max}$ are the minimum and maximum property operator p in HEN respectively.

The discretisation approach limits the search space of property operator p of hot stream h and cold stream c whose values are bounded between $\psi_{HEN,p}^{\min}$ and $\psi_{HEN,p}^{\max}$. Discretisation of the property operator p of hot stream h and cold stream c may be conducted in many ways. In this work, it is discretised based on property operator p of fresh resources, process sources and process sinks ($\psi_{r,p}, \psi_{i,p}$ and $\psi_{j,p}$) using the following notation:

$$\psi_{h,p} = \{\psi_{r,p},\ \psi_{i,p},\ \psi_{j,p}\} \tag{6.19}$$

$$\psi_{c,p} = \{\psi_{r,p},\ \psi_{i,p},\ \psi_{j,p}\} \tag{6.20}$$

Case study 3 with a single property operator is shown next to illustrate the concept, with limiting data given in Table 3.3. As shown, there are three sinks and three sources, with impurity concentration being the only property of concerned. The discretisation of impurity concentrations is first conducted. As shown in Table 3.3, the sets of operators for fresh resource, sources and sinks are given as ψ_r = {0 ppm}, ψ_i = {100 ppm, 800 ppm, 1100 ppm} and ψ_j = {50 ppm, 800 ppm}, respectively. Therefore, the property operators of both hot and cold streams are discretised as 0 ppm, 50 ppm, 100 ppm, 800 ppm and 1100 ppm. The intention is to reduce the number of discretisation values. Furthermore, it also reduces the piping needed for mixing and splitting of streams as compared to the *equal distribution method* proposed by Pham et al. (2009).

Step 2: Discretisation of temperatures for each hot stream h and cold stream c

Next, discretisation of supply and target temperatures of hot and cold streams (T_h^{in}, T_h^{out}, T_c^{in}, T_c^{out}) are conducted. The supply temperature of each stream is bounded by the temperatures of the sources; while the target temperature is bounded by the temperatures of the sinks. This results in $T_{\min}^{\text{in}} = \min\{T_i\}$, $T_{\max}^{\text{in}} = \max\{T_i\}$, $T_{\min}^{\text{out}} = \min\{T_j\}$ and $T_{\max}^{\text{out}} = \max\{T_j\}$. Then the boundaries for T_h^{in}, T_h^{out}, T_c^{in}, T_c^{out} are set as follows,

$$T_{\min}^{\text{in}} \le T_h^{\text{in}} \le T_{\max}^{\text{in}} \tag{6.21}$$

$$T_{\min}^{\text{in}} \le T_c^{\text{in}} \le T_{\max}^{\text{in}} \tag{6.22}$$

$$T_{\min}^{\text{out}} \le T_h^{\text{out}} \le T_{\max}^{\text{out}} \tag{6.23}$$

$$T_{\min}^{\text{out}} \le T_c^{\text{out}} \le T_{\max}^{\text{out}} \tag{6.24}$$

In order to reduce the size of the search space of the supply temperatures of hot and cold streams (T_h^{in} and T_c^{in}), the *convex hull approach* of Pham et al. (2009) is used. The main idea of this approach is that, the supply temperature of any hot and cold streams, which is a result of mixing of various process sources, will be enclosed in the convex hull constructed by the convex combination of the properties of the individual process sources. To illustrate this concept, the same Case study 3 in Table 3.3 is used. Without the convex hull approach, the original search space of the supply temperature of hot stream h is bounded by 0 ppm $\le \psi_h \le$ 1100 ppm and $20\,°C \le T_h^{\text{in}} \le 100\,°C$ (Figure 6.3(a)). Based on the data given in Table 3.3, all four process sources (SR1, SR2, SR3 and FW1) are allocated as dots on the search space.

Connecting these dots will then produce the convex hull (shaded area in Figure 6.3(b)) which is also referred to as the *attainable region* for hot stream *h*.

For the given flowrates of SR1, SR2, SR3 and FW1, any possible mixture will fall within the attainable region. Therefore, values outside the convex hull are not needed. The application of convex hull approach will significantly reduce the size of the search space. For the case in Figure 6.3, 52% reduction in search space has been achieved. This value is achieved by comparing the original search space region (Figure 6.3(a)) with attainable region after implementing convex hull approach (Figure 6.3(b)). The construction of convex hull is relatively simple for single property problem. However, it gets more challenging when more property operators are involved and may require convex hull algorithm from the field of geometrical mathematics such as the *Graham Scan Algorithm* (Graham, 1972).

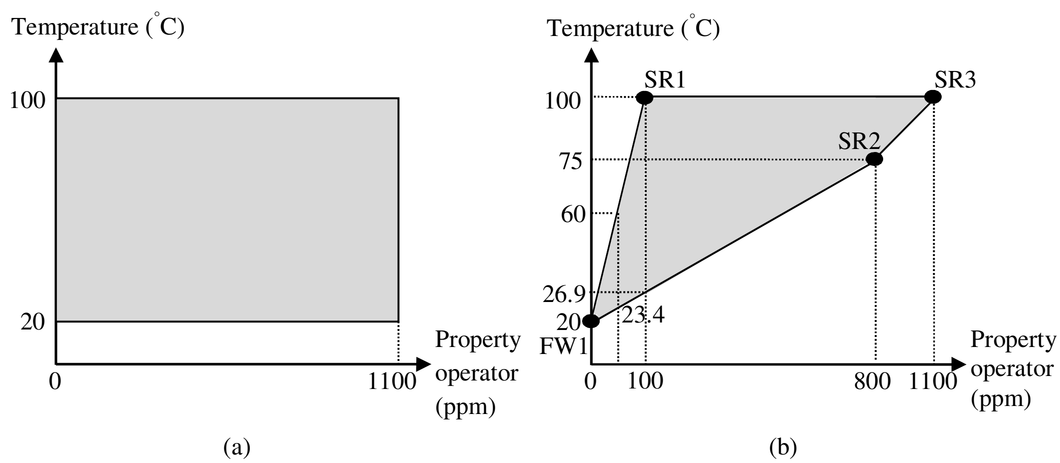


Figure 6.3: (a) Search space without convex hull approach. (b) Attainable region with convex hull approach.

Table 6.1 shows the supply and target temperature range for the hot and cold streams in Table 3.3. The supply temperature corresponding to each ψ is defined based on Figure 6.3(b), while the target temperature is bounded based on the process sink temperatures. For example, for ψ of 100 ppm, the corresponding T^{in}_{min} and T^{in}_{max} are obtained from the vertical dotted line at 100 ppm in Figure 6.3(b), which give 26.9°C and 100°C respectively. On the other hand, the corresponding T^{out}_{min} and T^{out}_{max} are based on the temperature of WW and SK1/SK3 in Table 3.3.

Table 6.1: Convex hull.

ψ (ppm)	T^{in}_{min} (°C)	T^{in}_{max} (°C)	T^{out}_{min} (°C)	T^{out}_{max} (°C)
0	20	20	30	100
50	23.4	60	30	100
100	26.9	100	30	100
800	75	100	30	100
1100	100	100	30	100

Based on the range defined in Table 6.2, one can now obtain the temperature range for hot (Table 6.2) and cold streams (Table 6.3) respectively. For example, for ψ of 0 ppm, the source can only be cold streams, as its supply temperature (20°C) is lower than the target temperature range (30 – 100°C). On the other hand, for ψ of 100 ppm, the temperature range in Table 6.1 allows hot streams to have $30\,°C \leq T_h^{in} \leq 100\,°C$ and $30\,°C \leq T_h^{out} \leq 100\,°C$ and cold streams with $26.9°C \leq T_c^{in} \leq 100\,°C$ and $30\,°C \leq T_c^{out} \leq 100\,°C$. With these defined range, these variables are then discretised based on the equal distribution method proposed by Pham et al. (2009). Note that more precise solution can be achieved with finer discretisation increments; however this will lead to larger model and computational expensive.

Table 6.2: Convex hull of hot streams.

ψ (ppm)	$T^{in}_{h,min}$ (°C)	$T^{in}_{h,max}$ (°C)	$T^{out}_{h,min}$ (°C)	$T^{out}_{h,max}$ (°C)
50	30	60	30	60
100	30	100	30	100
800	75	100	75	100
1100	100	100	30	100

Table 6.3: Convex hull of cold streams.

ψ (ppm)	$T_{c,\min}^{in}$ (°C)	$T_{c,\max}^{in}$ (°C)	$T_{c,\min}^{out}$ (°C)	$T_{c,\max}^{out}$ (°C)
0	20	20	30	100
50	23.4	60	30	100
100	26.9	100	30	100
800	75	100	75	100

Step 3: Application of integer cuts for hot and cold streams

It is computational expensive to have a large number of hot and cold streams. Therefore, the maximum number of hot stream *h* and cold stream *c* should be limited to *m*. To resolve this, integer cut technique as proposed by Pham et al. (2009) is used to select the desired number of hot stream *h* and cold stream *c*. Two binary variables ϕ_h and ϕ_c are introduced for hot stream *h* and cold stream *c* respectively. If a hot stream *h* or cold stream *c* is used in the solution, then its binary variable is assigned a value of 1 or else 0. The number of hot stream *h* and cold stream *c* is restricted by using the following linear constraints:

$$\sum_{i \in NSOURCES} w_{i,h} \leq U_h \phi_h \quad h \in NHOT \tag{6.25}$$

$$\sum_{i \in NSOURCES} w_{i,c} \leq U_c \phi_c \quad c \in NCOLD \tag{6.26}$$

$$\sum_{h \in NHOT} \phi_h + \sum_{c \in NCOLD} \phi_c \leq m \tag{6.27}$$

where U_h and U_c are the maximum flowrates of the hot stream *h* or cold stream *c*.

The presented solution strategy linearises the original proposed MINLP, which leads to an MILP model which can be solved easily using optimisation software such as LINGO.

6.6 Network configuration

Solving the proposed model for HIRCNs with heat of mixing will enable one to obtain a solution which consists of the minimum cost (AOC or TAC), the flowrate of fresh resources r, the external hot and cold utilities as well as the flowrate of each process stream in the source-HEN-sink superstructure. With these results, RCN configuration can be achieved. However, to achieve the complete HIRCN configuration, HEN design is also needed. As the solution only provides the external hot and cold utilities results, the HEN design will need to be synthesised using the classical *pinch design method* (Linnhoff and Flower, 1978a; Linnhoff et al., 1982; Smith, 2005). Furthermore, this HEN design can further verify the targeted results of hot and cold utilities in the solution.

6.7 Case studies

Case studies 3 and 4 presented in Chapter 3 are solved to demonstrate the proposed model. All case studies are solved using Extended LINGO v13.0 with Global Solver in a computer with a Core i3, 3.3 GHz processor. In all case studies, the costs of hot and cold utilities (Cost_h and Cost_c) are given as 3.758 \$/kW.h and 0.005 \$/kW.h respectively. In addition, total operating hour (k) and $\Delta T_{\min}$ are taken as 8000 h/y and 10°C respectively.

6.7.1 Case study 3

Case Study 3 reports a single property-based water network adopted from George et al. (2011). It consists of three process sinks and three process sources, with acetone and water in the process streams. The limiting data for this case study is given in Table 3.3. Fresh resource is pure fresh water (0 ppm), with unit cost of \$0.45/ton and is supplied at 20°C. On the other hand, wastewater has to be discharged at temperature of 30°C. In this case study, heat capacities of all streams (CP_c, CP_h, CP_i, CP_r and CP_j) are assumed to take a constant value of 4.2 kJ/kg.K as the process streams are mainly water.

The objective of this case study is to minimise the AOC, which consists of the operating costs for fresh resources, as well as hot and cold utilities in the HIRCN. The optimisation objective is given as follows:

$$\min_{F_r, Q_h, Q_c} AOC = k * \left\{ \sum_{r=1}^{NFRESH} \text{Cost}_r F_r + \text{Cost}_h Q_h + \text{Cost}_c Q_c \right\} \tag{6.28}$$

where Cost_r is the cost of fresh resources.

In this case study, the excess Gibbs free energy is estimated using the NRTL equation. The latter contains three parameters for a binary system and is written as

$$\frac{G^E}{x_1 x_2 RT} = \frac{G_{21}\tau_{21}}{x_1 + x_2 G_{21}} + \frac{G_{12}\tau_{12}}{x_2 + x_1 G_{12}} \tag{6.29}$$

with

$$G_{12} = \exp(-\alpha\tau_{12}) \tag{6.30}$$

$$G_{21} = \exp(-\alpha\tau_{21}) \tag{6.31}$$

$$\tau_{12} = \frac{d_{12}}{RT} \tag{6.32}$$

$$\tau_{21} = \frac{d_{21}}{RT} \tag{6.33}$$

where d_{12}, d_{21} and α are the parameters in NRTL equation. For acetone and water solution, these values are taken as 631.05, 1197.41 and 0.5343 respectively.

Equations 6.34 and 6.35 are the activity coefficients for the NRTL equation with binary systems.

$$\ln \gamma_1 = x_2^2 \left[\tau_{21} \left(\frac{G_{21}}{x_1 + x_2 G_{21}} \right)^2 + \frac{G_{12}\tau_{12}}{(x_2 + x_1 G_{12})^2} \right] \tag{6.34}$$

$$\ln \gamma_2 = x_1^2 \left[\tau_{12} \left(\frac{G_{12}}{x_2 + x_1 G_{12}} \right)^2 + \frac{G_{21}\tau_{21}}{(x_1 + x_2 G_{21})^2} \right] \tag{6.35}$$

In this case study, the maximum number of hot and cold streams, *m* is chosen as 3. Solving the optimisation objective in Equation 6.28, subject to the constraints in Equations 4.7 – 4.11, 4.16 – 4.20, 4.30, 6.1 – 6.15, 6.25 – 6.27 and 6.29 – 6.33, yield the minimum AOC of \$1,542,245 in 2 CPU minutes, with the optimal HIRCN shown in Figure 6.4. The values of F_r, Q_h and Q_c for the HIRCN are determined as 77.27 kg/s, 6,056.26 kW and 2,812.72 kW respectively with a true pinch point of 80ºC. To further verify the targeted results of Q_h and Q_c, the HEN for this case study is synthesised using the classical *pinch design method* (Linnhoff and Flower, 1978a; Linnhoff et al., 1982; Smith, 2005), and is presented in Figure 6.5. Note that the energy targets are identical as per that obtained via the proposed model. The LINGO code and solution for this case study can be found in Appendix E.

Note also that the AOC depends on the maximum number of hot and cold streams. There is an implied trader-off because the AOC may reduce if the maximum number of hot and cold streams increases as more streams are allocated for HEN, which may reduce the external hot and cold utilities needed; however, more heat exchangers may be needed, which leads to higher capital cost.

Sensitivity analysis is conducted to observe how maximum number of hot and cold streams affects the AOC. Figure 6.6 shows the plot of AOC versus maximum number of hot and cold streams for Case Study 3. As shown in the figure, as the maximum number of hot and cold streams increases, the AOC decreases proportionally and eventually level off when the maximum number of hot and cold streams reached 6. Figure 6.7 and Figure 6.8 show the optimal HIRCN and HEN with maximum number of hot and cold streams of 6, which are also the same results for maximum number of hot and cold streams of 7 and 8. The values of F_r, Q_h and Q_c

for this HIRCN are determined as 81.71 kg/s, 3442.95 kW and 13.21 kW respectively.

Comparing Figure 6.5 with Figure 6.8 it is noted that the larger maximum number of hot and cold streams is assigned, the more heat recovery can take place, which further reduce the hot and cold utilities, as well as the AOC. On the other hand, six additional heat exchangers are needed when the maximum number of hot and cold streams increases from 3 to 6. However, when the maximum number of hot and cold streams reaches 6, the heat recovery between hot and cold streams (which is constraint by the process sinks temperature) reaches its maximum. Therefore, a further increase of maximum number of hot and cold streams can no longer reduce the AOC, as no additional hot and cold streams is needed.

Furthermore, Case study 3 is also solved using the same model but without heat of mixing to demonstrate the impact of heat of mixing on the HIRCNs. To exclude heat of mixing in the HIRCN, additional constraints are added as follow,

$$\Delta H_c^{\mathrm{mix}} = 0 \quad c \in NCOLD \tag{6.36}$$

$$\Delta H_h^{\mathrm{mix}} = 0 \quad h \in NHOT \tag{6.37}$$

$$\Delta H_j^{\mathrm{mix}} = 0 \quad j \in NSINKS \tag{6.38}$$

$$\Delta H_{\mathrm{waste}}^{\mathrm{mix}} = 0 \tag{6.39}$$

Equation 6.28 is solved subject to constraints in Equations 4.7 – 4.16, 4.22, 5.1 – 5.3, 6.1 – 6.15, 6.25 – 6.27 and 6.36 – 6.39 with *m* value ranging from 3 to 8. The minimum AOC results for HIRCNs with and without heat of mixing are summarised in Table 6.4. As shown, HIRCNs with heat of mixing required a lower AOC as compared to HIRCNs without heat of mixing. This is mainly because when heat of mixing is considered for this case study, less flowrates are needed in the HEN due to energy generation at the mixing point. As a result of less flowrates in HEN, less external heating and cooling utilities as well as less fresh resources are needed. These can be verified by comparing the two HIRCNs and HENs in Figure 6.7 and Figure 6.8 with those in Figure 6.9 and Figure 6.10 for *m* of 6.

Table 6.4: Comparison of AOC for HIRCN with and without heat of mixing for Case Study 3.

m	AOC	
	HIRCN with heat of mixing	HIRCN without heat of mixing
3	1,542,245	1,542,355
4	1,383,700	1,383,822
5	1,335,634	1,335,752
6	1,334,614	1,334,732
7	1,334,614	1,334,732
8	1,334,614	1,334,732

6.7.2 Case study 4

A case study with only phenol and water in the process streams is solved to illustrate the proposed approach. This case study is adopted from Kheireddine et al. (2011), where multiple properties (concentration, temperature and vapour pressure) and heat of mixing are considered. Note that heat of mixing is temperature-dependent; while other properties are interdependence of temperature effect. Table 3.4 shows the limiting data for process sinks and sources as well as fresh resources for this case study. Note that two fresh resources are available to fulfill the process sinks requirement, i.e. pure fresh water (FR1) and fresh water with 0.012 mass fraction of impurity (FR2). The unit cost of these sources corresponds to \$0.00132/kg (FR1) and \$0.00088/kg (FR2) respectively.

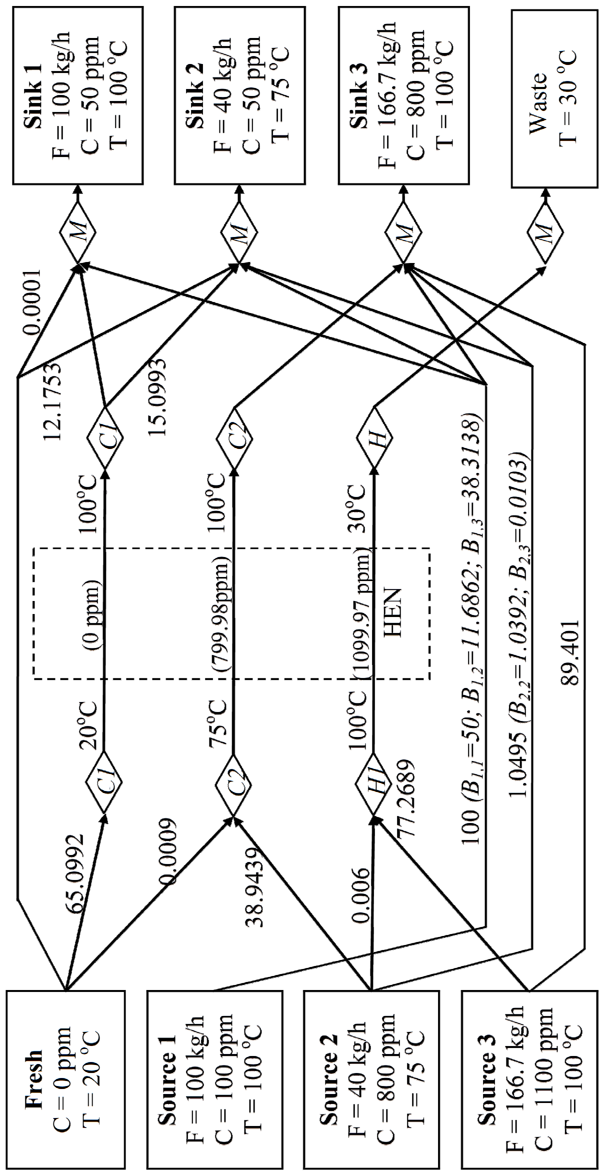


Figure 6.4: HIRCN with heat of mixing for Case Study 3 with m = 3.

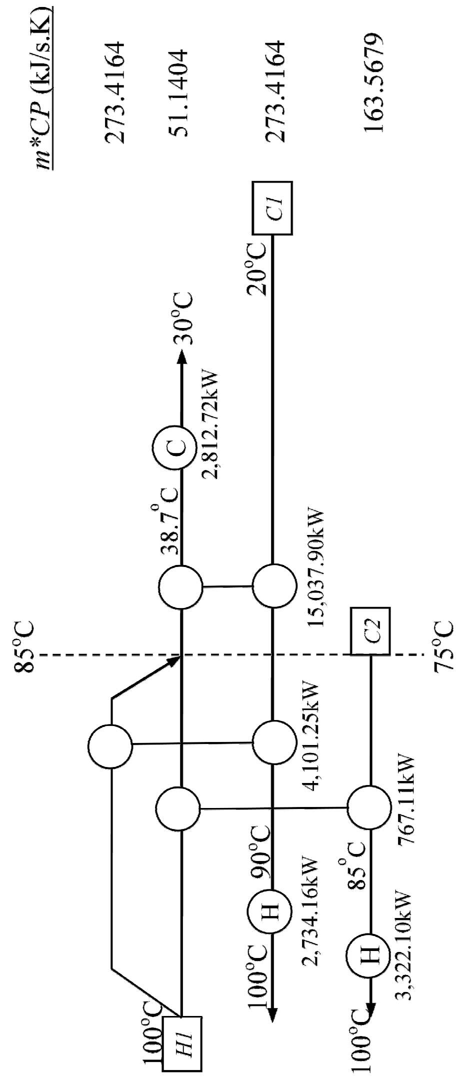


Figure 6.5: HEN for HIRCN with heat of mixing in Case Study 3 with $m = 3$.

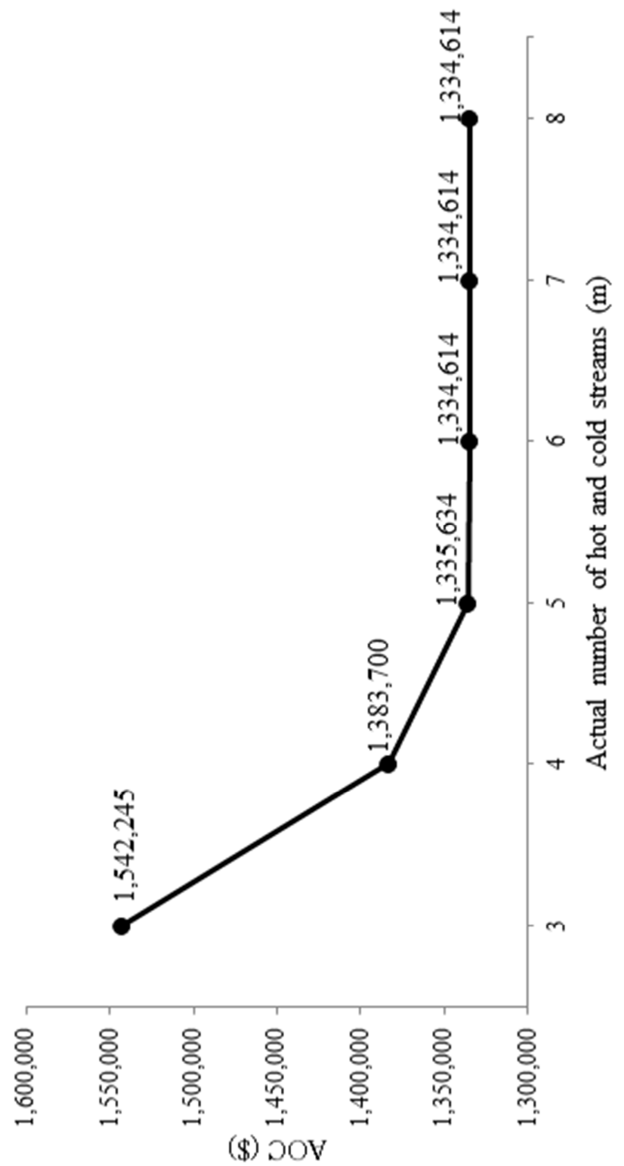
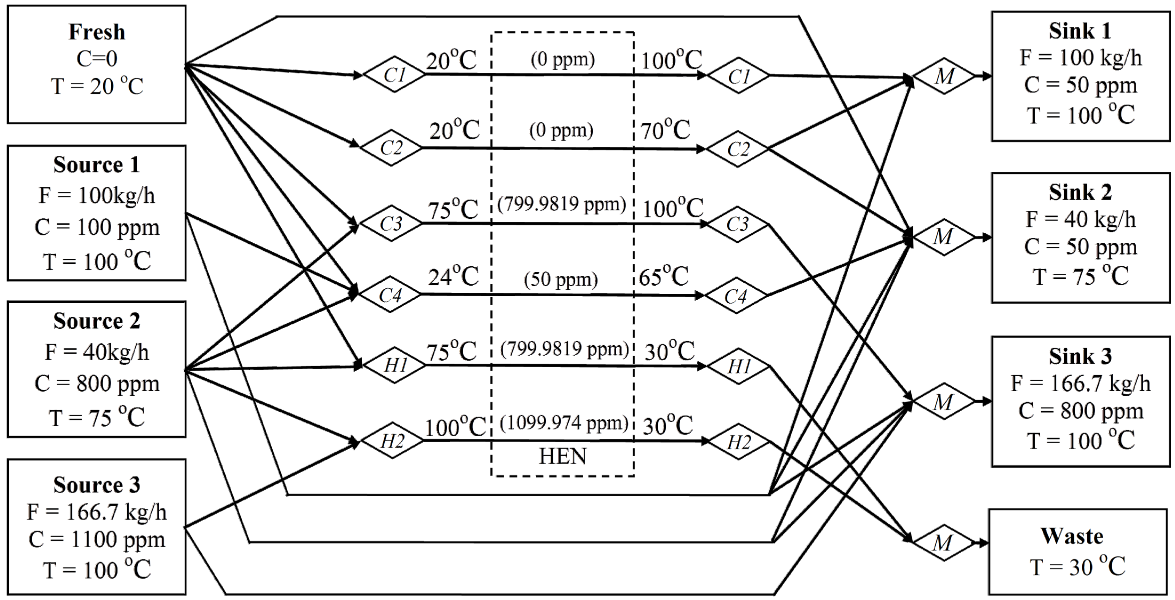


Figure 6.6: Sensitivity analysis for Case Study 3 - Effect of maximum number of hot and cold streams on



f **:** $f_{r,C1} = 49.9997$; $f_{r,C2} = 30.9202$; $f_{r,C3} = 0.0004$; $f_{r,C4} = 0.7320$; $f_{r,H1} = 0.0005$; $f_{r,2} = 0.0536$;

w **:** $w_{1,C4} = 0.0060$; $w_{2,C3} = 16.2462$; $w_{2,C4} = 0.0484$; $w_{2,H1} = 22.0657$; $w_{2,H2} = 0.0056$;

$w_{3,H2} = 65.4542$; $w_{1,1} = 50$; $w_{1,2} = 6.6163$; $w_{1,3} = 43.3776$; $w_{2,2} = 1.6238$; $w_{2,3} = 0.0103$;

$w_{3,3} = 101.2158$;

g **:** $g_{C1,1} = 49.9997$; $g_{C2,1} = 0.0032$; $g_{C2,2} = 30.9198$; $g_{C4,2} = 0.7865$; $g_{H1,3} = 22.0662$;

Figure 6.7: HIRCN with heat of mixing for Case Study 3 with $m = 6$.

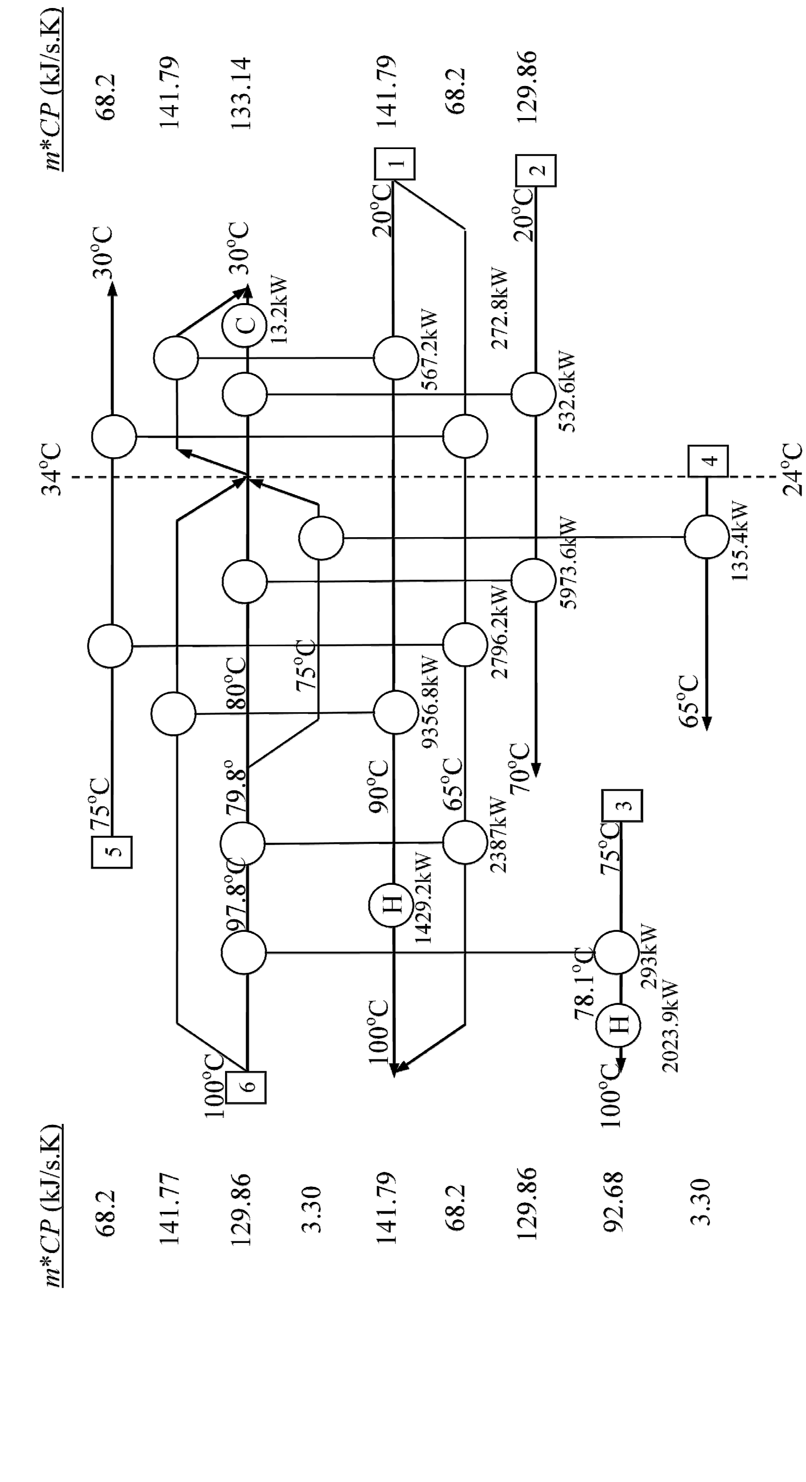


Figure 6.8: HEN for HIRCN with heat of mixing in Case Study 3 with $m = 6$.

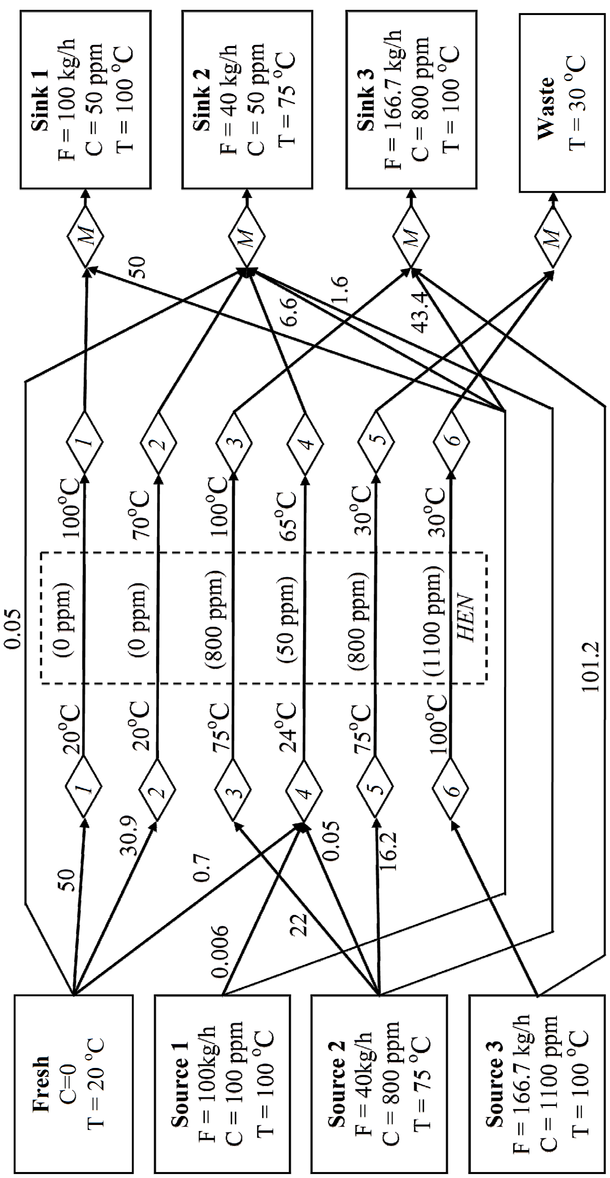


Figure 6.9: HIRCN without heat of mixing for Case Study 3 with $m = 6$.

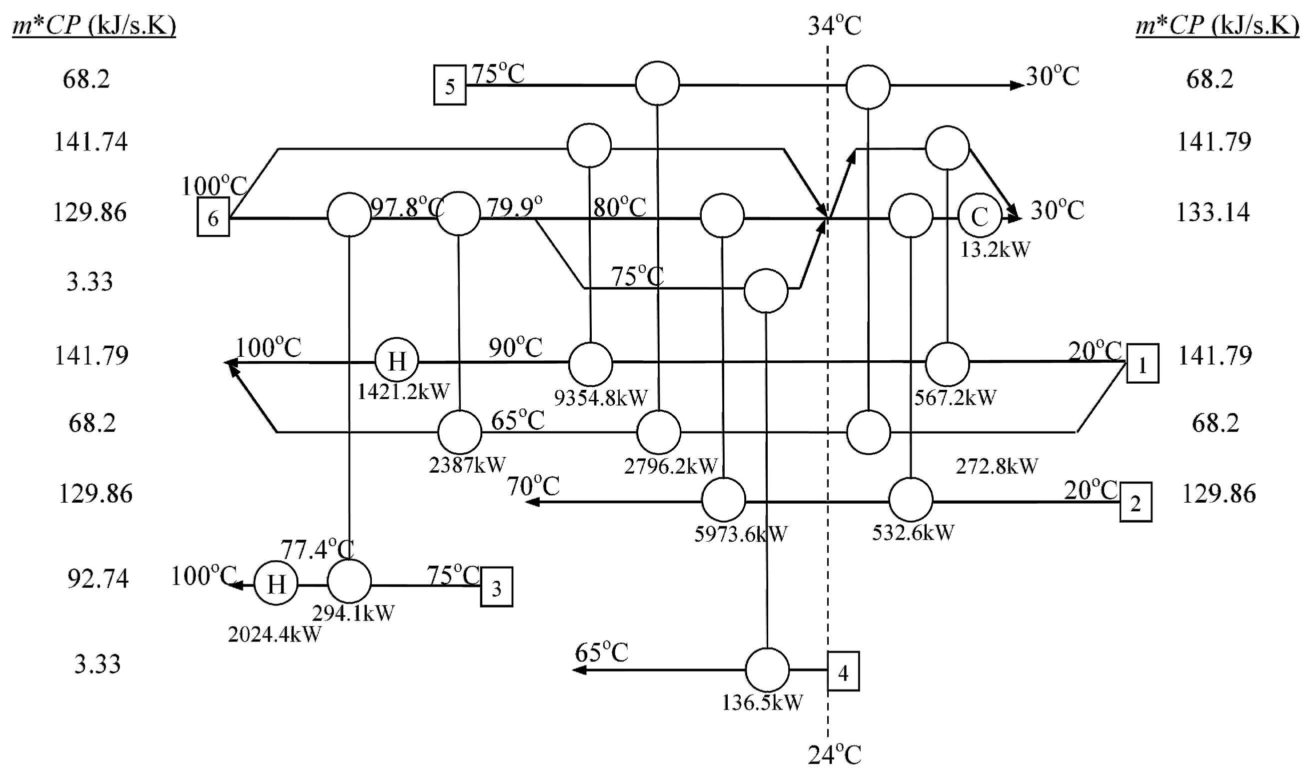


Figure 6.10: HEN for HIRCN without heat of mixing in Case Study 3 with m = 6.

In this case study, the Wilson equation is selected for the estimation of the excess Gibbs free energy. As the case study is a binary system, the Wilson equation contains only two binary parameters (Λ_{12} and Λ_{21}) and is expressed as

$$\frac{G^E}{RT} = -x_1 \ln(x_1 + x_2\Lambda_{12}) - x_2 \ln(x_2 + x_1\Lambda_{21}) \tag{6.40}$$

$$\ln \gamma_1 = -\ln(x_1 + x_2\Lambda_{12}) - x_2\left(\frac{\Lambda_{12}}{x_1 + x_2\Lambda_{12}} - \frac{\Lambda_{21}}{x_2 + x_1\Lambda_{21}}\right) \tag{6.41}$$

$$\ln \gamma_2 = -\ln(x_2 + x_1\Lambda_{21}) - x_1\left(\frac{\Lambda_{12}}{x_1 + x_2\Lambda_{12}} - \frac{\Lambda_{21}}{x_2 + x_1\Lambda_{21}}\right) \tag{6.42}$$

with

$$\ln \Lambda_{12} = a_{12} + \frac{b_{12}}{T} \tag{6.43}$$

$$\ln \Lambda_{21} = a_{21} + \frac{b_{21}}{T} \tag{6.44}$$

where a_{12}, a_{21}, b_{12} and b_{21} are the binary parameter in Wilson equation. For phenol and water solution, these values are taken as 2.4395, -3.2239, -2229.9297 and 1046.1246, respectively.

Hence, substituting Equation

$$\Delta H^{mix} = -Rx_1x_2\left(\frac{\Lambda_{12}b_{12}}{x_1 + x_2\Lambda_{12}} + \frac{\Lambda_{21}b_{21}}{x_2 + x_1\Lambda_{21}}\right) \tag{6.45}$$

Note that all the heat capacities in this case study can be determined via Equations 4.28 – 4.29 with the phenol and water parameters shown in Chapter 4.

The optimisation objective of this case study is to minimise AOC, which consists of operating costs for fresh resources, waste treatment as well as hot and cold utilities in the HIRCN, as shown in Equation 6.48.

$$\min_{F_r, F_w, Q_h, Q_c} AOC = k * \left\{ \sum_{r=1}^{NFRESH} Cost_r F_r + Cost_{waste} B^{waste} + Cost_h Q_h + Cost_c Q_c \right\} \tag{6.46}$$

where $Cost_{\mathrm{waste}}$ is the cost of waste and is taken as \$0.002/kg.

In this case study, the maximum number of hot and cold streams, m in Equation 6.31 is taken as 4. Equation 6.46 is solved subject to the constraints in Equations 4.7 – 4.11, 4.25 – 4.30, 4.36 – 4.37, 5.1 – 5.3, 6.1 – 6.15, 6.25 – 6.27, 6.43 – 6.44 and 6.45 with this m value. The minimum AOC of \$ 49,959 is determined in 4 CPU seconds with the optimised HIRCN presented in Figure 6.11. As shown, the synthesised HIRCN only consumes 1,234.1 kg/hr fresh resource 1 (FR1), without any utility needed. Furthermore, only two maximum number of hot and cold streams are needed. The HEN for this case study consist only one heat exchanger and is shown in Figure 6.11. The HEN is synthesised using the classical *pinch design method* (Linnhoff and Flower, 1978a; Linnhoff et al., 1982; Smith, 2005), which is also useful in order to verify the targeted results of Q_h and Q_c from the proposed model. Sensitivity analysis is conducted to observe how the maximum number of hot and cold streams affects the AOC (Figure 6.12). Only two hot and cold streams are needed for this case study. Note that the LINGO code and solution for this case study can be found in Appendix F.

6.8 Chapter summary

In this chapter, a novel methodology has been presented for the synthesis and optimisation of HIRCNs with heat of mixing. An MINLP formulation has been developed to identify the minimum cost of a HIRCN with heat of mixing as well as varying process parameters (e.g. flowrates, temperatures and properties). Since the model is nonlinear and non-convex, a discretisation approach has been proposed in this work to efficiently and effectively solve the optimisation problem. Two case studies are solved to illustrate the proposed approach.

Sensitivity analysis conducted in these case studies show that the larger maximum number of hot and cold streams are assigned, the more heat recovery could occur, which further reduce the hot and cold utilities as well as the AOC. On the other hand, additional heat exchangers are needed when the maximum number of hot and cold streams increases. However, when the maximum number of hot and cold streams reaches its optimal value, the heat recovery between hot and cold streams (which is constrained by the process sinks temperature) reaches its maximum. Therefore, a further increase of maximum number of hot and cold streams can no longer reduce the AOC, as no additional hot and cold streams is needed.

Moreover, one of the case studies presented had demonstrated that with consideration of heat of mixing, a lower AOC could be achieved. This is mainly because when heat of mixing is considered in this case study, less flowrates are needed in the HEN due to energy generation at the mixing point. Thus, less external heating and cooling utilities as well as less fresh resources are needed. Note that heat of mixing must be taken into consideration when liquid is involved in the process streams (i.e. gas-liquid mixture, liquid-liquid mixture or liquid-solid mixture). Heat of mixing can be ignored in cases with gas-gas mixture, gas-solid mixture and solid-solid mixture, or with dilute systems.

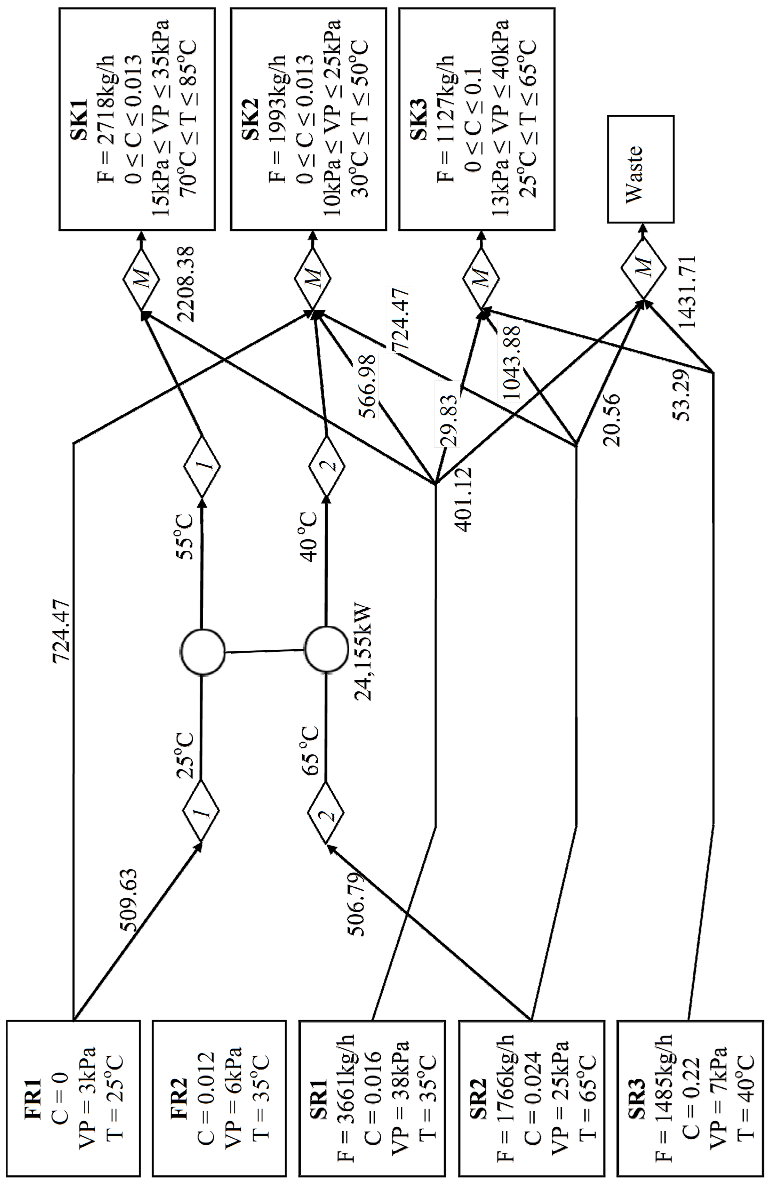


Figure 6.11: HIRCN with heat of mixing for Case Study 4 with m = 2

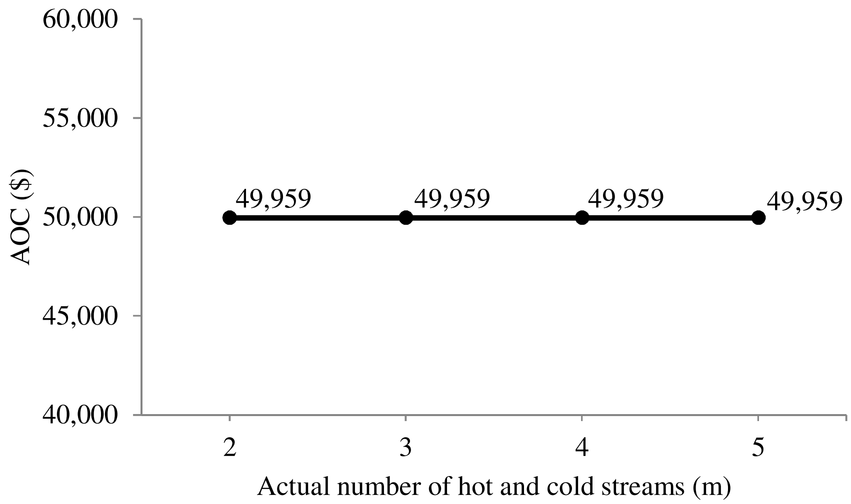


Figure 6.12: Sensitivity analysis for Case Study 4 - Effect of maximum number of hot and cold streams on AOC.

CHAPTER 7: CONCLUSIONS AND RECOMMENDATIONS FOR FUTURE WORK

7.1 Summary and significance

The work presented in this thesis offers some major contributions in the area of heat integrated resources conservation networks (HIRCNs). This work offers novel generic approaches for HIRCNs with and without heat of mixing that consider both concentration- and property-based systems.

A novel overall methodology for concentration- and property-based HIRCN synthesis has been established. This overall methodology provides guidance on the selection of the methodologies for HIRCNs with and without heat of mixing based on the type of mixtures in the process streams, as well as evaluation on whether the heat exchanger network (HEN) is needed in HIRCNs. On the other hand, a general framework for synthesis of HIRCNs with and without heat of mixing has been presented to strategically develop methodologies for HIRCNs with and without heat of mixing.

For utilities targeting in HENs with uncertain or varying range of flowrate and temperature, an improved mathematical model based on floating pinch concept has been developed and presented in this thesis. Stream location parameterisation for above and below pinch candidates have been explored. Besides, the model has been proven to be able to handle situations with temperature-dependent properties and varying operating parameters efficiently. This model has been used to determine the utilities targets in the methodologies for HIRCNs with and without heat of mixing.

A new methodology has been developed for the synthesis of HIRCNs without heat of mixing. The model formulation is complemented by the revised HEN floating pinch approach to determine the minimum cost of a HIRCN, which simultaneously optimised the fresh resources as well as the external hot and cold utilities. The model is able to solve for problems with varied process parameters. Moreover, comparison of the proposed model with two-stage optimisation approach has been addressed.

However, this methodology is not applicable for HIRCNs with heat of mixing as it may cause violation of the sink temperature constraint.

Thus, a new methodology for the synthesis of HIRCNs that encounter the effect of heat of mixing has been established to identify the minimum cost of HIRCN. The revised HEN floating pinch approach also has been utilised in this methodology. Besides, a discretisation approach has been proposed to guarantee solution quality and efficiency of the nonlinear and non-convex model. In addition, the interaction between the maximum number of hot and cold streams with heat recovery also has been explored. Moreover, it has been proven that lower HIRCN cost is achieved with consideration of heat of mixing.

7.2 Recommendations for future work

Since the work on concentration- and property-based HIRCNs is relatively new, three main areas for future developments are identified:

i. Synthesis of HIRCNs with piping and capital costs

   In this thesis, the HIRCNs methodologies presented have been mainly focused on minimising the annual operating cost, which are mainly cost for fresh resources as well as for energy utilities. The synthesis of HEN design is not solved simultaneously with the HIRCNs. Furthermore, the piping cost of HIRCNs is not included. All these may lead to expensive total annualised cost (including total operating and annualised capital costs) of a HIRCN. Thus, the trade-off between savings and investment should be considered simultaneously to identify an economical HIRCN.

ii. Synthesis of HIRCNs with regeneration and treatment systems

   Apart from considering reuse/recycle in the HIRCNs, the future work in HIRCNs includes incorporation of regeneration system in HIRCNs, which can further minimise the fresh resources consumption as well as the total operating cost of HIRCNs can be considered. Moreover, treatment systems can also be included to ensure that the waste discharged fulfilled the environmental regulations.

iii. Synthesis of HIRCNs for batch processes

In various industry sectors, such as food, pharmaceutical, biochemical manufacturing, processes are commonly operates in batch mode. To date, there is no work conducted on HIRCNs for batch process systems. The development of HIRCNs for batch process systems are industrially very common as well as important, hence is therefore required.

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APPENDIX A: HEN mathematical model and solution for Case study 5 in Chapter 4

Appendix A1 – HEN mathematical model for Case study 5

```
SETS:

JUNCTIONS_A/1..4/  : T_A;
JUNCTIONS_D/1..4/  : T_D;
HEN_1/1..2/        : T_AH_IN, T_AH_OUT, T_AC_IN, T_AC_OUT, MCPH_A,
                    MCPC_A;
PINCH_1/1..4/      : TP_A, A, B;
PINCH_BIN(HEN_1, PINCH_1): LAMSP, LAMTP, NSP, NTP;

ENDSETS

DATA:

T_A = 250 200 20 140;
T_D = 40 80 180 230;

ENDDATA

!Objective Function;
MIN = Qh;

!Minimum temperature difference;
DT = 10;

!Identifying (shifted temperatures) hot and cold streams;
T_AH_IN(1)   = T_A(1) - DT/2;
T_AH_OUT(1)  = T_D(1) - DT/2;
T_AH_IN(2)   = T_A(2) - DT/2;
T_AH_OUT(2)  = T_D(2) - DT/2;

T_AC_IN(1)   = T_A(3) + DT/2;
T_AC_OUT(1)  = T_D(3) + DT/2;
T_AC_IN(2)   = T_A(4) + DT/2;
T_AC_OUT(2)  = T_D(4) + DT/2;

!MCP values;
MCPH_A(1)  = 0.15;
MCPH_A(2)  = 0.25;
MCPC_A(1)  = 0.2;
MCPC_A(2)  = 0.3;

!Assigning pinch temperatures = supply temperatures;
TP_A(1)  = T_AH_IN(1);
TP_A(2)  = T_AH_IN(2);
TP_A(3)  = T_AC_IN(1);
TP_A(4)  = T_AC_IN(2);

!Identifying pinch location (BIN=1 below pinch, BIN=0, above pinch);
@FOR (PINCH_BIN(i, k):
      (0-TP_A(k))*LAMSP(i, k) < T_AH_IN(i)-TP_A(k);
      (10e6-TP_A(k))*(1-LAMSP(i, k)) >= T_AH_IN(i)-TP_A(k);
```

```
      (0-TP_A(k))*LAMTP(i, k) < T_AH_OUT(i)-TP_A(k);
      (10e6-TP_A(k))*(1-LAMTP(i, k)) >= T_AH_OUT(i)-TP_A(k);

      (0-TP_A(k))*NSP(i, k) < T_AC_IN(i)-TP_A(k);
      (10e6-TP_A(k))*(1-NSP(i, k)) >= T_AC_IN(i)-TP_A(k);

      (0-TP_A(k))*NTP(i, k) < T_AC_OUT(i)-TP_A(k);
      (10e6-TP_A(k))*(1-NTP(i, k)) >= T_AC_OUT(i)-TP_A(k));

@FOR (PINCH_1(k):
      @SUM(HEN_1(i):MCPH_A(i)*(LAMTP(i, k)*(TP_A(k)-T_AH_OUT(i))-
      LAMSP(i, k)*(TP_A(k)-T_AH_IN(i)))) = A(k);
      @SUM(HEN_1(j):MCPC_A(j)*(NSP(j, k)*(TP_A(k)-T_AC_IN(j))-NTP(j,
      k)*(TP_A(k)-T_AC_OUT(j)))) = B(k);
      A(k) - B(k) <= QC);

!Overall energy balance;
@SUM(HEN_1(i):MCPH_A(i)*(T_AH_IN(i)-T_AH_OUT(i))) -
@SUM(HEN_1(j):MCPC_A(j)*(T_AC_OUT(j)-T_AC_IN(j))) + QH - QC = 0;

!Defining binary integers;
@FOR (PINCH_BIN(i, k):@BIN(LAMTP(i, k)); @BIN(LAMSP(i, k));
@BIN(NTP(i, k)); @BIN(NSP(i, k)));

End
```

Appendix A2 – HEN solution for Case study 5

```
Global optimal solution found.
Objective value:                              7.500000
Objective bound:                              7.500000
Infeasibilities:                              0.000000
Extended solver steps:                               0
Total solver iterations:                             0

Model Class:                                      MILP

Total variables:                     42
Nonlinear variables:                  0
Integer variables:                   32

Total constraints:                   78
Nonlinear constraints:                0

Total nonzeros:                     115
Nonlinear nonzeros:                   0


    Variable           Value        Reduced Cost
          QH        7.500000            0.000000
          DT        10.00000            0.000000
          QC        10.00000            0.000000
     T_A( 1)        250.0000            0.000000
     T_A( 2)        200.0000            0.000000
     T_A( 3)        20.00000            0.000000
     T_A( 4)        140.0000            0.000000
     T_D( 1)        40.00000            0.000000
     T_D( 2)        80.00000            0.000000
     T_D( 3)        180.0000            0.000000
     T_D( 4)        230.0000            0.000000
 T_AH_IN( 1)        245.0000            0.000000
 T_AH_IN( 2)        195.0000            0.000000
T_AH_OUT( 1)        35.00000            0.000000
T_AH_OUT( 2)        75.00000            0.000000
 T_AC_IN( 1)        25.00000            0.000000
 T_AC_IN( 2)        145.0000            0.000000
T_AC_OUT( 1)        185.0000            0.000000
T_AC_OUT( 2)        235.0000            0.000000
  MCPH_A( 1)       0.1500000            0.000000
  MCPH_A( 2)       0.2500000            0.000000
  MCPC_A( 1)       0.2000000            0.000000
  MCPC_A( 2)       0.3000000            0.000000
    TP_A( 1)        245.0000            0.000000
    TP_A( 2)        195.0000            0.000000
    TP_A( 3)        25.00000            0.000000
    TP_A( 4)        145.0000            0.000000
       A( 1)        61.50000            0.000000
       A( 2)        54.00000            0.000000
       A( 3)        0.000000            0.000000
       A( 4)        34.00000            0.000000
       B( 1)        59.00000            0.000000
       B( 2)        47.00000            0.000000
       B( 3)        0.000000            0.000000
       B( 4)        24.00000            0.000000
LAMSP( 1, 1)        0.000000            0.000000
LAMSP( 1, 2)        0.000000            0.000000
```

```
LAMSP( 1, 3)        0.000000          0.000000
LAMSP( 1, 4)        0.000000          15.00000
LAMSP( 2, 1)        1.000000          0.000000
LAMSP( 2, 2)        0.000000          0.000000
LAMSP( 2, 3)        0.000000          0.000000
LAMSP( 2, 4)        0.000000          12.50000
LAMTP( 1, 1)        1.000000          0.000000
LAMTP( 1, 2)        1.000000          0.000000
LAMTP( 1, 3)        0.000000          0.000000
LAMTP( 1, 4)        1.000000          16.50000
LAMTP( 2, 1)        1.000000          0.000000
LAMTP( 2, 2)        1.000000          0.000000
LAMTP( 2, 3)        0.000000          0.000000
LAMTP( 2, 4)        1.000000          17.50000
  NSP( 1, 1)        1.000000          0.000000
  NSP( 1, 2)        1.000000          0.000000
  NSP( 1, 3)        0.000000          0.000000
  NSP( 1, 4)        1.000000         -24.00000
  NSP( 2, 1)        1.000000          0.000000
  NSP( 2, 2)        1.000000          0.000000
  NSP( 2, 3)        0.000000          0.000000
  NSP( 2, 4)        0.000000          0.000000
  NTP( 1, 1)        1.000000          0.000000
  NTP( 1, 2)        1.000000          0.000000
  NTP( 1, 3)        0.000000          0.000000
  NTP( 1, 4)        0.000000         -8.000000
  NTP( 2, 1)        1.000000          0.000000
  NTP( 2, 2)        0.000000          0.000000
  NTP( 2, 3)        0.000000          0.000000
  NTP( 2, 4)        0.000000         -27.00000
```

APPENDIX B: HEN mathematical model and solution for Case study 6 in Chapter 4

Appendix B1 – HEN mathematical model for Case study 6

```
SETS:

JUNCTIONS_A/1..4/  :  T_A, A_Cp, A_Cp_water, A_Cp_phenol, X_water,
                   X_phenol, Cp;
JUNCTIONS_D/1..4/  :  T_D, D_Cp, D_Cp_water, D_Cp_phenol;
HEN_1/1..2/        : T_AH_IN, T_AH_OUT, T_AC_IN, T_AC_OUT, MCPH_A,
                   MCPC_A, MH, MC;
PINCH_1/1..4/      : TP_A, A, B;
PINCH_BIN(HEN_1, PINCH_1): LAMSP, LAMTP, NSP, NTP;

ENDSETS

!Temperature range;
@BND(160, T_A(1),160);
@BND( 80, T_A(2),80);
@BND( 50, T_A(3),50);
@BND( 80, T_A(4),80);
@BND( 40, T_D(1), 40);
@BND( 60, T_D(2), 60);
@BND(115, T_D(3),115);
@BND(220, T_D(4),220);

!MCP values;
@BND (0.010, MH(1), 0.020);
@BND (0.010, MH(2) , 0.020);
@BND (0.005, MC(1) , 0.010);
@BND (0.015, MC(2), 0.020);

!Objective Functions;
MIN = Qh;

!Minimum temperature difference;
DT = 10;

!Identifying (shifted temperatures) hot and cold streams;
T_AH_IN(1) = T_A(1) - DT/2;
T_AH_OUT(1) = T_D(1) - DT/2;
T_AH_IN(2) = T_A(2) - DT/2;
T_AH_OUT(2) = T_D(2) - DT/2;

T_AC_IN(1) = T_A(3) + DT/2;
T_AC_OUT(1) = T_D(3) + DT/2;
T_AC_IN(2) = T_A(4) + DT/2;
T_AC_OUT(2) = T_D(4) + DT/2;

MCPH_A(1) = Cp(1)*MH(1);
MCPH_A(2) = Cp(2)*MH(2);
MCPC_A(1) = Cp(3)*MC(1);
MCPC_A(2) = Cp(4)*MC(2);
```

```
!Cp calculation ;
X_water(1) = 0.995;
X_water(2) = 0.998;
X_water(3) = 0.940;
X_water(4) = 0.978;
X_phenol(1) = 1 - X_water(1);
X_phenol(2) = 1 - X_water(2);
X_phenol(3) = 1 - X_water(3);
X_phenol(4) = 1 - X_water(4);

@FOR(JUNCTIONS_A(i):A_Cp(i) = X_water(i)*A_Cp_water(i) +
X_phenol(i)*A_Cp_phenol(i)); !J/g.K;
@FOR(JUNCTIONS_A(i):A_Cp_water(i)  = 1.3724 + 0.0083 * T_A(i)+273));
                              !J/g.K;
@FOR(JUNCTIONS_A(i):A_Cp_phenol(i) = 0.4685 + 0.0044 * T_A(i)+273));
                              !J/g.K;

@FOR(JUNCTIONS_D(i):D_Cp(i) = X_water(i)*D_Cp_water(i) +
X_phenol(i)*D_Cp_phenol(i)); !J/g.K;
@FOR(JUNCTIONS_D(i):D_Cp_water(i)  = 1.3724 + 0.0083 * T_D(i)+273));
                              !J/g.K;
@FOR(JUNCTIONS_D(i):D_Cp_phenol(i) = 0.4685 + 0.0044 * T_D(i)+273));
                              !J/g.K;

2*Cp(1) = A_Cp(1) + D_Cp(1);
2*Cp(2) = A_Cp(2) + D_Cp(2);
2*Cp(3) = A_Cp(3) + D_Cp(3);
2*Cp(4) = A_Cp(4) + D_Cp(4);

!Assigning pinch temperatures = supply temperatures;
TP_A(1) = T_AH_IN(1);
TP_A(2) = T_AH_IN(2);
TP_A(3) = T_AC_IN(1);
TP_A(4) = T_AC_IN(2);

!Identifying pinch location (BIN=1 below pinch, BIN=0, above pinch);
@FOR (PINCH_BIN(i, k):
      (0-TP_A(k))*LAMSP(i, k) < T_AH_IN(i)-TP_A(k);
      (10e6-TP_A(k))*(1-LAMSP(i, k)) >= T_AH_IN(i)-TP_A(k);

      (0-TP_A(k))*LAMTP(i, k) < T_AH_OUT(i)-TP_A(k);
      (10e6-TP_A(k))*(1-LAMTP(i, k)) >= T_AH_OUT(i)-TP_A(k);

      (0-TP_A(k))*NSP(i, k) < T_AC_IN(i)-TP_A(k);
      (10e6-TP_A(k))*(1-NSP(i, k)) >= T_AC_IN(i)-TP_A(k);

      (0-TP_A(k))*NTP(i, k) < T_AC_OUT(i)-TP_A(k);
      (10e6-TP_A(k))*(1-NTP(i, k)) >= T_AC_OUT(i)-TP_A(k));

@FOR (PINCH_1(k):
      @SUM(HEN_1(i):MCPH_A(i)*(LAMTP(i, k)*(TP_A(k)-T_AH_OUT(i))-
      LAMSP(i, k)*(TP_A(k)-T_AH_IN(i)))) = A(k);
      @SUM(HEN_1(j):MCPC_A(j)*(NSP(j, k)*(TP_A(k)-T_AC_IN(j))-NTP(j,
      k)*(TP_A(k)-T_AC_OUT(j)))) = B(k);
      A(k) - B(k) <= QC);

!Overall energy balance;
@SUM(HEN_1(i):MCPH_A(i)*(T_AH_IN(i)-T_AH_OUT(i))) -
@SUM(HEN_1(j):MCPC_A(j)*(T_AC_OUT(j)-T_AC_IN(j))) + QH - QC = 0;
```

```
!Defining binary integers;
@FOR (PINCH_BIN(i, k):@BIN(LAMTP(i, k)); @BIN(LAMSP(i, k));
@BIN(NTP(i, k)); @BIN(NSP(i, k)));

End
```

Appendix B2 – HEN solution for Case study 6

```
Global optimal solution found.
  Objective value:                              5.068477
  Objective bound:                              5.068477
  Infeasibilities:                              0.000000
  Total solver iterations:                             0

  Model Class:                                     MINLP

  Total variables:                    98
  Nonlinear variables:                56
  Integer variables:                  32

  Total constraints:                 122
  Nonlinear constraints:              77

  Total nonzeros:                    419
  Nonlinear nonzeros:                236


       Variable           Value        Reduced Cost
             QH        5.068477            0.000000
             DT        10.00000            0.000000
             QC        4.296071            0.000000
        T_A( 1)        160.0000          -0.7240698E-01
        T_A( 2)        80.00000            0.000000
        T_A( 3)        50.00000            0.000000
        T_A( 4)        80.00000           0.4312438E-02
       A_CP( 1)        4.953337            0.000000
       A_CP( 2)        4.297739            0.000000
       A_CP( 3)        3.923484            0.000000
       A_CP( 4)        4.252127            0.000000
 A_CP_WATER( 1)        4.966300            0.000000
 A_CP_WATER( 2)        4.302300            0.000000
 A_CP_WATER( 3)        4.053300            0.000000
 A_CP_WATER( 4)        4.302300            0.000000
A_CP_PHENOL( 1)        2.373700            0.000000
A_CP_PHENOL( 2)        2.021700            0.000000
A_CP_PHENOL( 3)        1.889700            0.000000
A_CP_PHENOL( 4)        2.021700            0.000000
    X_WATER( 1)       0.9950000            0.000000
    X_WATER( 2)       0.9980000            0.000000
    X_WATER( 3)       0.9400000            0.000000
    X_WATER( 4)       0.9780000            0.000000
   X_PHENOL( 1)       0.5000000E-02        0.000000
   X_PHENOL( 2)       0.2000000E-02        0.000000
   X_PHENOL( 3)       0.6000000E-01        0.000000
   X_PHENOL( 4)       0.2200000E-01        0.000000
         CP( 1)        4.456507            0.000000
         CP( 2)        4.214817            0.000000
         CP( 3)        4.185629            0.000000
         CP( 4)        4.827121            0.000000
        T_D( 1)        40.00000            0.000000
        T_D( 2)        60.00000            0.000000
        T_D( 3)        115.0000            0.000000
        T_D( 4)        220.0000           0.7671919E-01
       D_CP( 1)        3.959677            0.000000
       D_CP( 2)        4.131895            0.000000
       D_CP( 3)        4.447774            0.000000
```

```
        D_CP( 4)        5.402115            0.000000
  D_CP_WATER( 1)        3.970300            0.000000
  D_CP_WATER( 2)        4.136300            0.000000
  D_CP_WATER( 3)        4.592800            0.000000
  D_CP_WATER( 4)        5.464300            0.000000
 D_CP_PHENOL( 1)        1.845700            0.000000
 D_CP_PHENOL( 2)        1.933700            0.000000
 D_CP_PHENOL( 3)        2.175700            0.000000
 D_CP_PHENOL( 4)        2.637700            0.000000
     T_AH_IN( 1)        155.0000            0.000000
     T_AH_IN( 2)        75.00000            0.000000
    T_AH_OUT( 1)        35.00000            0.000000
    T_AH_OUT( 2)        55.00000            0.000000
     T_AC_IN( 1)        55.00000            0.000000
     T_AC_IN( 2)        85.00000            0.000000
    T_AC_OUT( 1)        120.0000            0.000000
    T_AC_OUT( 2)        225.0000            0.000000
      MCPH_A( 1)       0.8913014E-01        0.000000
      MCPH_A( 2)       0.4214817E-01        0.000000
      MCPC_A( 1)       0.3344666E-01        0.000000
      MCPC_A( 2)       0.7240681E-01        0.000000
          MH( 1)       0.2000000E-01      -0.8467360E-03
          MH( 2)       0.1000000E-01      -0.4214814E-03
          MC( 1)       0.7990831E-02        0.000000
          MC( 2)       0.1500000E-01        337.8985
        TP_A( 1)        155.0000            0.000000
        TP_A( 2)        75.00000            0.000000
        TP_A( 3)        55.00000            0.000000
        TP_A( 4)        85.00000            0.000000
           A( 1)        11.53858            0.000000
           A( 2)        4.408169            0.000000
           A( 3)        1.782603            0.000000
           A( 4)        5.299470            0.000000
           B( 1)        7.242509            0.000000
           B( 2)       0.6689331            0.000000
           B( 3)        0.000000            0.000000
           B( 4)        1.003400            0.000000
    LAMSP( 1, 1)        0.000000            0.000000
    LAMSP( 1, 2)        0.000000            0.000000
    LAMSP( 1, 3)        0.000000            0.000000
    LAMSP( 1, 4)        0.000000           0.6239110E-05
    LAMSP( 2, 1)        1.000000           -6.743700
    LAMSP( 2, 2)        0.000000            0.000000
    LAMSP( 2, 3)        0.000000            0.000000
    LAMSP( 2, 4)        1.000000          -0.8429634E-06
    LAMTP( 1, 1)        1.000000            10.69561
    LAMTP( 1, 2)        1.000000            0.000000
    LAMTP( 1, 3)        1.000000            0.000000
    LAMTP( 1, 4)        1.000000           0.4456507E-05
    LAMTP( 2, 1)        1.000000            8.429625
    LAMTP( 2, 2)        1.000000            0.000000
    LAMTP( 2, 3)        0.000000            0.000000
    LAMTP( 2, 4)        1.000000           0.2528890E-05
      NSP( 1, 1)        1.000000           -3.344642
      NSP( 1, 2)        1.000000            0.000000
      NSP( 1, 3)        0.000000            0.000000
      NSP( 1, 4)        1.000000          -0.1003394E-05
      NSP( 2, 1)        1.000000           -5.068472
      NSP( 2, 2)        0.000000            0.000000
      NSP( 2, 3)        0.000000            0.000000
      NSP( 2, 4)        0.000000            0.000000
```

```
NTP( 1, 1)        1.000000          1.170625
NTP( 1, 2)        0.000000          0.000000
NTP( 1, 3)        0.000000          0.000000
NTP( 1, 4)        0.000000         -0.1170626E-05
NTP( 2, 1)        0.000000         -5.068472
NTP( 2, 2)        0.000000          0.000000
NTP( 2, 3)        0.000000          0.000000
NTP( 2, 4)        0.000000         -0.1013695E-04
```

APPENDIX C: HIRCN mathematical model for Case study 1 in Chapter 5

Appendix C1 – HIRCN mathematical model for Case study 1

```
SETS:

HOT/1..8/      :Th_s, Th_t, Cph, Fh, Cost_h, Th_s_data, Th_t_data;
COLD/1..16/    :Tc_s, Tc_t, Cpc, Fc, Cost_c, Tc_s_data, Tc_t_data;
PINCH/1..24/   :T_p, A, B;
HP(HOT,PINCH) :Lamtp, Lamsp;
CP(COLD,PINCH):Ntp, Nsp;
Source/1..4/   :FR, CR, WW;
Sink/1..4/     :FK, CK, AA;
Connection (Source,Sink):F;
ENERGY/1..5/   :Q;

ENDSETS

DATA:

!Supply and target temperatures;
Th_s_data = 30 43 43 130 130 130 130 35;
Tc_s_data = 30 30 30 21 21 21 21 21 43 43 43 130 35 35 35 35;
Th_t_data = 30 30 40 30 55 98 40 30;
Tc_t_data = 187 55 98 30 187 55 98 40 187 55 98 187 187 55 98 40;

!Flowrate of sources;
FR = 530 68 1130 36;

!Flowrate of sinks;
FK = 350 677 126 202;

!Concentration of sources;
CR = 30 150 300 500;

!Constraints of sink inlet mass fraction;
CK = 0 40 75 100;
ENDDATA

!Target temperatures;
Tout_data1 =  30;
Tout_data2 = 187;
Tout_data3 =  55;
Tout_data4 =  98;
Tout_data5 =  40;

!Information needed;
DT = 35;
Heat_capacity = 2.19; !kJ/kg.K;

!Shifted temperatures;
@FOR(HOT(i): Th_s(i)  = Th_s_data(i)  - DT/2);
@FOR(HOT(i): Th_t(i)  = Th_t_data(i)  - DT/2);
@FOR(COLD(j):Tc_s(j)  = Tc_s_data(j)  + DT/2);
@FOR(COLD(j):Tc_t(j)  = Tc_t_data(j)  + DT/2);
```

```
!Pinch temperature = Supply temperature;
T_p(1) = Th_s(1) ;
T_p(2) = Th_s(2) ;
T_p(3) = Th_s(3) ;
T_p(4) = Th_s(4) ;
T_p(5) = Th_s(5) ;
T_p(6) = Th_s(6) ;
T_p(7) = Th_s(7) ;
T_p(8) = Th_s(8) ;
T_p(9) = Tc_s(1) ;
T_p(10) = Tc_s(2) ;
T_p(11) = Tc_s(3) ;
T_p(12) = Tc_s(4) ;
T_p(13) = Tc_s(5) ;
T_p(14) = Tc_s(6) ;
T_p(15) = Tc_s(7) ;
T_p(16) = Tc_s(8) ;
T_p(17) = Tc_s(9) ;
T_p(18) = Tc_s(10) ;
T_p(19) = Tc_s(11) ;
T_p(20) = Tc_s(12) ;
T_p(21) = Tc_s(13) ;
T_p(22) = Tc_s(14) ;
T_p(23) = Tc_s(15) ;
T_p(24) = Tc_s(16) ;

!Relate CP = FCp;
@FOR(HOT(i): Cph(i) = Fh(i)*Heat_capacity);
@FOR(COLD(j): Cpc(j) = Fc(j)*Heat_capacity);

!Selection of hot or cold flowrate;
AA(1)  = 350;
Fh(1)  = 0;

AA(2)  = Fc(1);
AA(3)  = Fc(2);
AA(4)  = Fc(3);

F(1,1) = Fc(4);
F(1,2) = Fc(5);
F(1,3) = Fc(6);
F(1,4) = Fc(7);
WW(1)  = Fc(8);

F(2,1) = Fh(2);
F(2,2) = Fc(9);
F(2,3) = Fc(10);
F(2,4) = Fc(11);
WW(2)  = Fh(3);

F(3,1) = Fh(4);
F(3,2) = Fc(12);
F(3,3) = Fh(5);
F(3,4) = Fh(6);
WW(3)  = Fh(7);

F(4,1) = Fh(8);
F(4,2) = Fc(13);
F(4,3) = Fc(14);
F(4,4) = Fc(15);
WW(4)  = Fc(16);
```

```
!Calculate total energy received by each sink;
Q(1) = Fh(1)*Th_t_data(1) + Fc(4)*Tc_t_data(4) + Fh(2)*Th_t_data(2)
+ Fh(4)*Th_t_data(4) + Fh(8)*Th_t_data(8);

Q(2) = Fc(1)*Tc_t_data(1) + Fc(5)*Tc_t_data(5) + Fc(9)*Tc_t_data(9)
+ Fc(12)*Tc_t_data(12) + Fc(13)*Tc_t_data(13);

Q(3) = Fc(2)*Tc_t_data(2) + Fc(6)*Tc_t_data(6) +
Fc(10)*Tc_t_data(10) + Fh(5)*Th_t_data(5) + Fc(14)*Tc_t_data(14);

Q(4) = Fc(3)*Tc_t_data(3) + Fc(7)*Tc_t_data(7) +
Fc(11)*Tc_t_data(11) + Fh(6)*Th_t_data(6) + Fc(15)*Tc_t_data(15);

Q(5) = Fc(8)*Tc_t_data(8) + Fh(3)*Th_t_data(3) + Fh(7)*Th_t_data(7)
+ Fc(16)*Tc_t_data(16);

Fsk1 = F(1,1) + AA(1) + F(2,1) + F(3,1) + F(4,1);
Fsk2 = F(1,2) + AA(2) + F(2,2) + F(3,2) + F(4,2);
Fsk3 = F(1,3) + AA(3) + F(2,3) + F(3,3) + F(4,3);
Fsk4 = F(1,4) + AA(4) + F(2,4) + F(3,4) + F(4,4);
Fsk5 = WW(1) + WW(2) + WW(3) + WW(4);

!Calculate Tsink based on reuse/recycle stremas;
Tout_data1 = Q1 /(Fsk1);
Tout_data2 = Q2 /(Fsk2);
Tout_data3 = Q3 /(Fsk3);
Tout_data4 = Q4 /(Fsk4);
Tout_data5 = Q5 /(Fsk5);

!Objective function = minimise operation cost;
MIN = Total_AA*Cost_AA + Qc*Cost_CW + Qh*Cost_HH;

Cost_AA = 14400000; !$/yr;
Cost_CW = 20; !$/yr;
Cost_HH = 80;!$/yr;

!Total fresh AA and WW;
Total_AA = @SUM(Sink(i):AA(i));
Total_WW = @SUM(Source(j):WW(j));

!Sink flowrate balance;
@FOR(Sink(j):FK(j) = AA(j) + @SUM(Source(i):F(i,j)));

!Source flowrate balance;
@FOR(Source(i):FR(i) = @SUM(Sink(j):F(i,j)) + WW(i));

!Sink mass load balance;
@FOR(Sink(j):@SUM(Connection(i,j):F(i,j)*CR(i)) <= FK(j)*CK(j));

!Overall energy balance;
@SUM(HOT(i):Cph(i)*(Th_s(i)-Th_t(i)))-@SUM(COLD(j):Cpc(j)*(Tc_t(j)-
Tc_s(j)))+ Qh - Qc = 0;

!To identify the pinch location;
@FOR(PINCH(k): @SUM(HOT(i):Cph(i)*((Lamtp(i,k)*(T_p(k)-Th_t(i)))-
Lamsp(i,k)*(T_p(k)-Th_s(i))))=A(k));
@FOR(PINCH(k):@SUM(COLD(j):Cpc(j)*((Nsp(j,k)*(T_p(k)-Tc_s(j)))-
Ntp(j,k)*(T_p(k)-Tc_t(j))))    =B(k));
@FOR(PINCH(k):A(k) - B(k) - Qc <= 0);
```

```
!Linearlisation for binary integer;
@FOR(HP(i,k):((0 - T_p(k))* Lamtp(i,k)) - (Th_t(i) - T_p(k))
<0 );

@FOR(HP(i,k):(Th_t(i) - T_p(k)) - ((1000000-T_p(k))*(1-
Lamtp(i,k)))<=0);

@FOR(HP(i,k):((0 - T_p(k))* Lamsp(i,k)) - (Th_s(i) - T_p(k))
<0);

@FOR(HP(i,k):(Th_s(i) - T_p(k)) - ((1000000-T_p(k))*(1-
Lamsp(i,k)))<=0);

@FOR(CP(j,k):((0 - T_p(k))* Ntp(j,k)) - (Tc_t(j) - T_p(k))
<0) ;

@FOR(CP(j,k):(Tc_t(j) - T_p(k)) - ((1000000-T_p(k))*(1-Ntp(j,k)))
<=0);

@FOR(CP(j,k):((0 - T_p(k))* Nsp(j,k)) - (Tc_s(j) - T_p(k))
<0);

@FOR(CP(j,k):(Tc_s(j) - T_p(k)) - ((1000000-T_p(k))*(1-Nsp(j,k)))
<=0);

!Binary integer;
@FOR(HP(i,k):@BIN(Lamtp(i,k));@BIN(Lamsp(i,k)));
@FOR(CP(j,k):@BIN(Ntp(j,k)); @BIN(Nsp(j,k)));

END
```

Appendix C2 – HIRCN solution for Case study 1

```
Global optimal solution found.
  Objective value:                              0.9442779E+10
  Objective bound:                              0.9442779E+10
  Infeasibilities:                               0.000000
  Extended solver steps:                                0
  Total solver iterations:                            196

  Model Class:                                      MINLP

  Total variables:                   1327
  Nonlinear variables:               1050
  Integer variables:                 1157

  Total constraints:                 2453
  Nonlinear constraints:               53

  Total nonzeros:                    4243
  Nonlinear nonzeros:                1579

            Variable           Value
          TOUT_DATA1        30.00000
          TOUT_DATA2        187.0000
          TOUT_DATA3        55.00000
          TOUT_DATA4        98.00000
          TOUT_DATA5        40.00000
                  DT        35.00000
       HEAT_CAPACITY        2.190000
                FSK1        350.0000
                FSK2        677.0000
                FSK3        126.0000
                FSK4        202.0000
                FSK5        1063.900
                  Q1        10500.00
                  Q2        126599.0
                  Q3        6930.000
                  Q4        19796.00
                  Q5        42556.00
            TOTAL_AA        654.9000
             COST_AA       0.1440000E+08
                  QC        79228.16
             COST_CW        20.00000
                  QH        132927.0
             COST_HH        80.00000
            TOTAL_WW        1063.900
            TH_S( 1)        12.50000
            TH_S( 2)        25.50000
            TH_S( 3)        25.50000
            TH_S( 4)        112.5000
            TH_S( 5)        112.5000
            TH_S( 6)        112.5000
            TH_S( 7)        112.5000
            TH_S( 8)        17.50000
            TH_T( 1)        12.50000
            TH_T( 2)        12.50000
            TH_T( 3)        22.50000
            TH_T( 4)        12.50000
            TH_T( 5)        37.50000
            TH_T( 6)        80.50000
            TH_T( 7)        22.50000
```

```
      TH_T( 8)        12.50000
       CPH( 1)        0.000000
       CPH( 2)        0.000000
       CPH( 3)        0.000000
       CPH( 4)        0.000000
       CPH( 5)        0.000000
       CPH( 6)        94.49444
       CPH( 7)        2251.101
       CPH( 8)        0.000000
        FH( 1)        0.000000
        FH( 2)        0.000000
        FH( 3)        0.000000
        FH( 4)        0.000000
        FH( 5)        0.000000
        FH( 6)        43.14815
        FH( 7)        1027.900
        FH( 8)        0.000000
    COST_H( 1)        0.000000
    COST_H( 2)        0.000000
    COST_H( 3)        0.000000
    COST_H( 4)        0.000000
    COST_H( 5)        0.000000
    COST_H( 6)        0.000000
    COST_H( 7)        0.000000
    COST_H( 8)        0.000000
 TH_S_DATA( 1)        30.00000
 TH_S_DATA( 2)        43.00000
 TH_S_DATA( 3)        43.00000
 TH_S_DATA( 4)        130.0000
 TH_S_DATA( 5)        130.0000
 TH_S_DATA( 6)        130.0000
 TH_S_DATA( 7)        130.0000
 TH_S_DATA( 8)        35.00000
 TH_T_DATA( 1)        30.00000
 TH_T_DATA( 2)        30.00000
 TH_T_DATA( 3)        40.00000
 TH_T_DATA( 4)        30.00000
 TH_T_DATA( 5)        55.00000
 TH_T_DATA( 6)        98.00000
 TH_T_DATA( 7)        40.00000
 TH_T_DATA( 8)        30.00000
      TC_S( 1)        47.50000
      TC_S( 2)        47.50000
      TC_S( 3)        47.50000
      TC_S( 4)        38.50000
      TC_S( 5)        38.50000
      TC_S( 6)        38.50000
      TC_S( 7)        38.50000
      TC_S( 8)        38.50000
      TC_S( 9)        60.50000
     TC_S( 10)        60.50000
     TC_S( 11)        60.50000
     TC_S( 12)        147.5000
     TC_S( 13)        52.50000
     TC_S( 14)        52.50000
     TC_S( 15)        52.50000
     TC_S( 16)        52.50000
      TC_T( 1)        204.5000
      TC_T( 2)        72.50000
      TC_T( 3)        115.5000
      TC_T( 4)        47.50000
```

```
      TC_T( 5)         204.5000
      TC_T( 6)         72.50000
      TC_T( 7)         115.5000
      TC_T( 8)         57.50000
      TC_T( 9)         204.5000
     TC_T( 10)         72.50000
     TC_T( 11)         115.5000
     TC_T( 12)         204.5000
     TC_T( 13)         204.5000
     TC_T( 14)         72.50000
     TC_T( 15)         115.5000
     TC_T( 16)         57.50000
       CPC( 1)         667.7310
       CPC( 2)         0.000000
       CPC( 3)         0.000000
       CPC( 4)         0.000000
       CPC( 5)         685.7944
       CPC( 6)         172.4625
       CPC( 7)         302.4431
       CPC( 8)         0.000000
       CPC( 9)         0.000000
      CPC( 10)         103.4775
      CPC( 11)         45.44250
      CPC( 12)         129.1046
      CPC( 13)         0.000000
      CPC( 14)         0.000000
      CPC( 15)         0.000000
      CPC( 16)         78.84000
        FC( 1)         304.9000
        FC( 2)         0.000000
        FC( 3)         0.000000
        FC( 4)         0.000000
        FC( 5)         313.1481
        FC( 6)         78.75000
        FC( 7)         138.1019
        FC( 8)         0.000000
        FC( 9)         0.000000
       FC( 10)         47.25000
       FC( 11)         20.75000
       FC( 12)         58.95185
       FC( 13)         0.000000
       FC( 14)         0.000000
       FC( 15)         0.000000
       FC( 16)         36.00000
    COST_C( 1)         0.000000
    COST_C( 2)         0.000000
    COST_C( 3)         0.000000
    COST_C( 4)         0.000000
    COST_C( 5)         0.000000
    COST_C( 6)         0.000000
    COST_C( 7)         0.000000
    COST_C( 8)         0.000000
    COST_C( 9)         0.000000
   COST_C( 10)         0.000000
   COST_C( 11)         0.000000
   COST_C( 12)         0.000000
   COST_C( 13)         0.000000
   COST_C( 14)         0.000000
   COST_C( 15)         0.000000
   COST_C( 16)         0.000000
 TC_S_DATA( 1)         30.00000
```

```
 TC_S_DATA( 2)        30.00000
 TC_S_DATA( 3)        30.00000
 TC_S_DATA( 4)        21.00000
 TC_S_DATA( 5)        21.00000
 TC_S_DATA( 6)        21.00000
 TC_S_DATA( 7)        21.00000
 TC_S_DATA( 8)        21.00000
 TC_S_DATA( 9)        43.00000
TC_S_DATA( 10)        43.00000
TC_S_DATA( 11)        43.00000
TC_S_DATA( 12)        130.0000
TC_S_DATA( 13)        35.00000
TC_S_DATA( 14)        35.00000
TC_S_DATA( 15)        35.00000
TC_S_DATA( 16)        35.00000
 TC_T_DATA( 1)        187.0000
 TC_T_DATA( 2)        55.00000
 TC_T_DATA( 3)        98.00000
 TC_T_DATA( 4)        30.00000
 TC_T_DATA( 5)        187.0000
 TC_T_DATA( 6)        55.00000
 TC_T_DATA( 7)        98.00000
 TC_T_DATA( 8)        40.00000
 TC_T_DATA( 9)        187.0000
TC_T_DATA( 10)        55.00000
TC_T_DATA( 11)        98.00000
TC_T_DATA( 12)        187.0000
TC_T_DATA( 13)        187.0000
TC_T_DATA( 14)        55.00000
TC_T_DATA( 15)        98.00000
TC_T_DATA( 16)        40.00000
       T_P( 1)        12.50000
       T_P( 2)        25.50000
       T_P( 3)        25.50000
       T_P( 4)        112.5000
       T_P( 5)        112.5000
       T_P( 6)        112.5000
       T_P( 7)        112.5000
       T_P( 8)        17.50000
       T_P( 9)        47.50000
       T_P( 10)        47.50000
       T_P( 11)        47.50000
       T_P( 12)        38.50000
       T_P( 13)        38.50000
       T_P( 14)        38.50000
       T_P( 15)        38.50000
       T_P( 16)        38.50000
       T_P( 17)        60.50000
       T_P( 18)        60.50000
       T_P( 19)        60.50000
       T_P( 20)        147.5000
       T_P( 21)        52.50000
       T_P( 22)        52.50000
       T_P( 23)        52.50000
       T_P( 24)        52.50000
          A( 1)        0.000000
          A( 2)        6753.303
          A( 3)        6753.303
          A( 4)        205622.9
          A( 5)        205622.9
          A( 6)        205622.9
```

A(7)	205622.9
A(8)	0.000000
A(9)	56277.52
A(10)	56277.52
A(11)	56277.52
A(12)	36017.62
A(13)	36017.62
A(14)	36017.62
A(15)	36017.62
A(16)	36017.62
A(17)	85541.84
A(18)	85541.84
A(19)	85541.84
A(20)	205622.9
A(21)	67533.03
A(22)	67533.03
A(23)	67533.03
A(24)	67533.03
B(1)	0.000000
B(2)	0.000000
B(3)	0.000000
B(4)	126394.8
B(5)	126394.8
B(6)	126394.8
B(7)	126394.8
B(8)	0.000000
B(9)	10446.30
B(10)	10446.30
B(11)	10446.30
B(12)	0.000000
B(13)	0.000000
B(14)	0.000000
B(15)	0.000000
B(16)	0.000000
B(17)	34610.10
B(18)	34610.10
B(19)	34610.10
B(20)	174811.8
B(21)	19588.46
B(22)	19588.46
B(23)	19588.46
B(24)	19588.46
LAMTP(1, 1)	0.000000
LAMTP(1, 2)	1.000000
LAMTP(1, 3)	1.000000
LAMTP(1, 4)	1.000000
LAMTP(1, 5)	1.000000
LAMTP(1, 6)	1.000000
LAMTP(1, 7)	1.000000
LAMTP(1, 8)	1.000000
LAMTP(1, 9)	1.000000
LAMTP(1, 10)	1.000000
LAMTP(1, 11)	1.000000
LAMTP(1, 12)	1.000000
LAMTP(1, 13)	1.000000
LAMTP(1, 14)	1.000000
LAMTP(1, 15)	1.000000
LAMTP(1, 16)	1.000000
LAMTP(1, 17)	1.000000
LAMTP(1, 18)	1.000000
LAMTP(1, 19)	1.000000

```
LAMTP( 1, 20)         1.000000
LAMTP( 1, 21)         1.000000
LAMTP( 1, 22)         1.000000
LAMTP( 1, 23)         1.000000
LAMTP( 1, 24)         1.000000
 LAMTP( 2, 1)         0.000000
 LAMTP( 2, 2)         1.000000
 LAMTP( 2, 3)         1.000000
 LAMTP( 2, 4)         1.000000
 LAMTP( 2, 5)         1.000000
 LAMTP( 2, 6)         1.000000
 LAMTP( 2, 7)         1.000000
 LAMTP( 2, 8)         1.000000
 LAMTP( 2, 9)         1.000000
LAMTP( 2, 10)         1.000000
LAMTP( 2, 11)         1.000000
LAMTP( 2, 12)         1.000000
LAMTP( 2, 13)         1.000000
LAMTP( 2, 14)         1.000000
LAMTP( 2, 15)         1.000000
LAMTP( 2, 16)         1.000000
LAMTP( 2, 17)         1.000000
LAMTP( 2, 18)         1.000000
LAMTP( 2, 19)         1.000000
LAMTP( 2, 20)         1.000000
LAMTP( 2, 21)         1.000000
LAMTP( 2, 22)         1.000000
LAMTP( 2, 23)         1.000000
LAMTP( 2, 24)         1.000000
 LAMTP( 3, 1)         0.000000
 LAMTP( 3, 2)         1.000000
 LAMTP( 3, 3)         1.000000
 LAMTP( 3, 4)         1.000000
 LAMTP( 3, 5)         1.000000
 LAMTP( 3, 6)         1.000000
 LAMTP( 3, 7)         1.000000
 LAMTP( 3, 8)         0.000000
 LAMTP( 3, 9)         1.000000
LAMTP( 3, 10)         1.000000
LAMTP( 3, 11)         1.000000
LAMTP( 3, 12)         1.000000
LAMTP( 3, 13)         1.000000
LAMTP( 3, 14)         1.000000
LAMTP( 3, 15)         1.000000
LAMTP( 3, 16)         1.000000
LAMTP( 3, 17)         1.000000
LAMTP( 3, 18)         1.000000
LAMTP( 3, 19)         1.000000
LAMTP( 3, 20)         1.000000
LAMTP( 3, 21)         1.000000
LAMTP( 3, 22)         1.000000
LAMTP( 3, 23)         1.000000
LAMTP( 3, 24)         1.000000
 LAMTP( 4, 1)         0.000000
 LAMTP( 4, 2)         1.000000
 LAMTP( 4, 3)         1.000000
 LAMTP( 4, 4)         1.000000
 LAMTP( 4, 5)         1.000000
 LAMTP( 4, 6)         1.000000
 LAMTP( 4, 7)         1.000000
 LAMTP( 4, 8)         1.000000
```

```
 LAMTP( 4, 9)         1.000000
LAMTP( 4, 10)         1.000000
LAMTP( 4, 11)         1.000000
LAMTP( 4, 12)         1.000000
LAMTP( 4, 13)         1.000000
LAMTP( 4, 14)         1.000000
LAMTP( 4, 15)         1.000000
LAMTP( 4, 16)         1.000000
LAMTP( 4, 17)         1.000000
LAMTP( 4, 18)         1.000000
LAMTP( 4, 19)         1.000000
LAMTP( 4, 20)         1.000000
LAMTP( 4, 21)         1.000000
LAMTP( 4, 22)         1.000000
LAMTP( 4, 23)         1.000000
LAMTP( 4, 24)         1.000000
 LAMTP( 5, 1)         0.000000
 LAMTP( 5, 2)         0.000000
 LAMTP( 5, 3)         0.000000
 LAMTP( 5, 4)         1.000000
 LAMTP( 5, 5)         1.000000
 LAMTP( 5, 6)         1.000000
 LAMTP( 5, 7)         1.000000
 LAMTP( 5, 8)         0.000000
 LAMTP( 5, 9)         1.000000
LAMTP( 5, 10)         1.000000
LAMTP( 5, 11)         1.000000
LAMTP( 5, 12)         1.000000
LAMTP( 5, 13)         1.000000
LAMTP( 5, 14)         1.000000
LAMTP( 5, 15)         1.000000
LAMTP( 5, 16)         1.000000
LAMTP( 5, 17)         1.000000
LAMTP( 5, 18)         1.000000
LAMTP( 5, 19)         1.000000
LAMTP( 5, 20)         1.000000
LAMTP( 5, 21)         1.000000
LAMTP( 5, 22)         1.000000
LAMTP( 5, 23)         1.000000
LAMTP( 5, 24)         1.000000
 LAMTP( 6, 1)         0.000000
 LAMTP( 6, 2)         0.000000
 LAMTP( 6, 3)         0.000000
 LAMTP( 6, 4)         1.000000
 LAMTP( 6, 5)         1.000000
 LAMTP( 6, 6)         1.000000
 LAMTP( 6, 7)         1.000000
 LAMTP( 6, 8)         0.000000
 LAMTP( 6, 9)         0.000000
LAMTP( 6, 10)         0.000000
LAMTP( 6, 11)         0.000000
LAMTP( 6, 12)         0.000000
LAMTP( 6, 13)         0.000000
LAMTP( 6, 14)         0.000000
LAMTP( 6, 15)         0.000000
LAMTP( 6, 16)         0.000000
LAMTP( 6, 17)         0.000000
LAMTP( 6, 18)         0.000000
LAMTP( 6, 19)         0.000000
LAMTP( 6, 20)         1.000000
LAMTP( 6, 21)         0.000000
```

```
LAMTP( 6, 22)         0.000000
LAMTP( 6, 23)         0.000000
LAMTP( 6, 24)         0.000000
 LAMTP( 7, 1)         0.000000
 LAMTP( 7, 2)         1.000000
 LAMTP( 7, 3)         1.000000
 LAMTP( 7, 4)         1.000000
 LAMTP( 7, 5)         1.000000
 LAMTP( 7, 6)         1.000000
 LAMTP( 7, 7)         1.000000
 LAMTP( 7, 8)         0.000000
 LAMTP( 7, 9)         1.000000
LAMTP( 7, 10)         1.000000
LAMTP( 7, 11)         1.000000
LAMTP( 7, 12)         1.000000
LAMTP( 7, 13)         1.000000
LAMTP( 7, 14)         1.000000
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 LAMSP( 1, 9)         1.000000
LAMSP( 1, 10)         1.000000
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LAMSP( 3, 23)        1.000000
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     NTP( 16, 13)        0.000000
     NTP( 16, 14)        0.000000
     NTP( 16, 15)        0.000000
     NTP( 16, 16)        0.000000
     NTP( 16, 17)        1.000000
     NTP( 16, 18)        1.000000
     NTP( 16, 19)        1.000000
     NTP( 16, 20)        1.000000
     NTP( 16, 21)        0.000000
     NTP( 16, 22)        0.000000
     NTP( 16, 23)        0.000000
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       NSP( 1, 3)        0.000000
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      NSP( 2, 20)        1.000000
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   NSP( 16, 15)        0.000000
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   NSP( 16, 18)        1.000000
   NSP( 16, 19)        1.000000
   NSP( 16, 20)        1.000000
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   NSP( 16, 23)        0.000000
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          H( 1)        0.000000
          H( 2)        0.000000
          H( 3)        0.000000
          H( 4)        0.000000
          H( 5)        0.000000
         FR( 1)        530.0000
         FR( 2)        68.00000
         FR( 3)        1130.000
         FR( 4)        36.00000
         CR( 1)        30.00000
         CR( 2)        150.0000
         CR( 3)        300.0000
         CR( 4)        500.0000
         WW( 1)        0.000000
         WW( 2)        0.000000
         WW( 3)        1027.900
         WW( 4)        36.00000
         FK( 1)        350.0000
         FK( 2)        677.0000
         FK( 3)        126.0000
         FK( 4)        202.0000
         CK( 1)        0.000000
         CK( 2)        40.00000
         CK( 3)        75.00000
         CK( 4)        100.0000
         AA( 1)        350.0000
```

```
      AA( 2)        304.9000
      AA( 3)        0.000000
      AA( 4)        0.000000
    F( 1, 1)        0.000000
    F( 1, 2)        313.1481
    F( 1, 3)        78.75000
    F( 1, 4)        138.1019
    F( 2, 1)        0.000000
    F( 2, 2)        0.000000
    F( 2, 3)        47.25000
    F( 2, 4)        20.75000
    F( 3, 1)        0.000000
    F( 3, 2)        58.95185
    F( 3, 3)        0.000000
    F( 3, 4)        43.14815
    F( 4, 1)        0.000000
    F( 4, 2)        0.000000
    F( 4, 3)        0.000000
    F( 4, 4)        0.000000
      TS( 1)        0.000000
      TS( 2)        0.000000
      TS( 3)        0.000000
      TS( 4)        0.000000
      TS( 5)        0.000000
      TT( 1)        0.000000
      TT( 2)        0.000000
      TT( 3)        0.000000
      TT( 4)        0.000000
      TT( 5)        0.000000
       Q( 1)        0.000000
       Q( 2)        126599.0
       Q( 3)        6930.000
       Q( 4)        19796.00
       Q( 5)        42556.00
```

APPENDIX D: HIRCN mathematical model and solution for Case study 2 in Chapter 5

Appendix D1 – HIRCN solution for Case study 2

```
SETS:

HOT/1..5/      :Th_s, Th_t, Cph, Fh, Cost_h, Th_s_data, Th_t_data;
COLD/1..4/     :Tc_s, Tc_t, Cpc, Fc, Cost_c, Tc_s_data, Tc_t_data;
PINCH/1..9/    :T_p, A, B;
HP(HOT,PINCH) :Lamtp, Lamsp;
CP(COLD,PINCH):Ntp, Nsp;
Source/1..2/   :FR, CR, WW, ToxR, THODR, pHR, DR, VR;
Sink/1..2/     :FK, CK, AA, ToxK, THODK, pHK, DK, VK;
Connection (Source,Sink):F;
ENERGY/1..8/   :Q;

ENDSETS

DATA:

!Supply temperatures;
Th_s_data = 160 160 120 160 120; !in oC;
Tc_s_data = 160 120 25 25; !in oC;
!Flowrate of sources;
FR = 2900 2450;
!Flowrate of sinks;
FK = 3000 1900;
!Concentration of sources;
CR = 0.033 0.022;
!Toxicity of sources;
ToxR = 0.8 0.5;
!THOD of sources;
THODR = 75 88;
!pH of sources;
pHR = 5.3 5.1;
!Density of sources;
DR = 2.000 2.208;
!Viscosity of sources;
VR = 1.256 1.220;

ENDDATA

!Constraints of sink inlet mass fraction;
CK(1) >= 0;
CK(1) <= 0.013;
CK(2) >= 0;
CK(2) <= 0.011;

!Constraints of sink inlet toxicity;
ToxK(1) >= 0;
ToxK(1) <= 2;
ToxK(2) >= 0;
ToxK(2) <= 2;
```

```
!Constraints of sink inlet THOD;
THODK(1) >= 0;
THODK(1) <= 75;
THODK(2) >= 0;
THODK(2) <= 75;

!Constraints of sink inlet pH;
pHK(1) >= 5.9;
pHK(1) <= 8;
pHK(2) >= 5.7;
pHK(2) <= 7.9;

!Constraints of sink inlet density;
DK(1) >= 1.8;
DK(1) <= 2.8;
DK(2) >= 1.7;
DK(2) <= 2.5;

!Constraints of sink inlet viscosity;
VK(1) >= 0.871;
VK(1) <= 1.202;
VK(2) >= 0.782;
VK(2) <= 1.43;

!Fresh data;
CA = 0;
ToxA = 0;
THODA = 0;
pHA = 7;
DA = 2.204;
VA = 1.002;

!Target temperatures;
@BND(130, Tout_data1, 180);
@BND( 60, Tout_data2, 110);
@BND( 27, Tout_w,      35);

!Boundaries of Target temperatures;
@BND(130, Th_t_data(1), 159);
@BND( 60, Th_t_data(2), 110);
@BND( 60, Th_t_data(3), 110);
@BND( 27, Th_t_data(4),  35);
@BND( 27, Th_t_data(5),  35);

@BND(161, Tc_t_data(1), 180);
@BND(130, Tc_t_data(2), 180);
@BND(130, Tc_t_data(3), 180);
@BND( 60, Tc_t_data(4), 110);

!Objective function = minimise operation cost;
MIN = Total_AA*Cost_AA + Qc*Cost_CW + Qh*Cost_HH;

Cost_AA = 72;    !$/yr
Cost_CW = 0.012; !$/yr;
Cost_HH = 5.269; !$/yr;

!Total fresh AA and WW;
Total_AA = AA(1) + AA(2);
Total_WW = WW(1) + WW(2);
```

```
!Sink flowrate balance;
@FOR(Sink(j):FK(j) = AA(j) + @SUM(Source(i):F(i,j)));

!Source flowrate balance;
FR(1) = F(1,1) + F(1,2) + WW(1);
FR(2) = F(2,1) + F(2,2) + WW(2);

!Sink composition balance;
@FOR(Sink(j):@SUM(Connection(i,j):F(i,j)*CR(i)) + AA(j)*CA <=
FK(j)*CK(j));

!Sink toxicity balance;
@FOR(Sink(j):@SUM(Connection(i,j):F(i,j)*ToxR(i)) + AA(j)*ToxA <=
FK(j)*ToxK(j));

!Sink THOD balance;
@FOR(Sink(j):@SUM(Connection(i,j):F(i,j)*THODR(i)) + AA(j)*THODA <=
FK(j)*THODK(j));

!Sink pH balance;
@FOR(Sink(j):@SUM(Connection(i,j):F(i,j)*10^(-pHR(i))) + AA(j)*10^(-
pHA) <= FK(j)*10^(-pHK(j)));

!Sink density balance;
@FOR(Sink(j):@SUM(Connection(i,j):F(i,j)*1/DR(i)) + AA(j)*1/DA <=
FK(j)*1/DK(j));

!Sink viscosity balance;
@FOR(Sink(j):@SUM(Connection(i,j):F(i,j)*@LOG(VR(i))) +
AA(j)*@LOG(VA) <= FK(j)*@LOG(VK(j)));

DT = 10;
Heat_capacity = 1.7976; !Btu/lb.C = 4.1813kJ/kg.K for water;

!Shifted temperatures;
@FOR(HOT(i): Th_s(i) = Th_s_data(i) - DT/2);
@FOR(HOT(i): Th_t(i) = Th_t_data(i) - DT/2);
@FOR(COLD(j):Tc_s(j) = Tc_s_data(j) + DT/2);
@FOR(COLD(j):Tc_t(j) = Tc_t_data(j) + DT/2);

!Pinch temperature = Supply temperature;
T_p(1) = Th_s(1);
T_p(2) = Th_s(2);
T_p(3) = Th_s(3);
T_p(4) = Th_s(4);
T_p(5) = Th_s(5);

T_p(6) = Tc_s(1);
T_p(7) = Tc_s(2);
T_p(8) = Tc_s(3);
T_p(9) = Tc_s(4);

!Relate CP = FCp;
@FOR(HOT(i): Cph(i) = Fh(i)*Heat_capacity);
@FOR(COLD(j): Cpc(j) = Fc(j)*Heat_capacity);

!Identification of hot and cold flowrate;
F(1,1) = Fh(1) + Fc(1);
F(1,2) = Fh(2);
AA(1)  = Fc(3);
AA(2)  = Fc(4);
```

```
F(2,1)  = Fc(2);
F(2,2)  = Fh(3);
WW(1)   = Fh(4);
WW(2)   = Fh(5);

!Calculate total energy received by each sink;
Q(1) = (Fh(1)*Th_t_data(1)*Heat_capacity) +
(Fc(1)*Tc_t_data(1)*Heat_capacity);
Q(2) = (Fh(2)*Th_t_data(2)*Heat_capacity) ;
Q(3) = (Fc(3)*Tc_t_data(3)*Heat_capacity) ;
Q(4) = (Fc(4)*Tc_t_data(4)*Heat_capacity) ;
Q(5) = (Fc(2)*Tc_t_data(2)*Heat_capacity) ;
Q(6) = (Fh(3)*Th_t_data(3)*Heat_capacity) ;
Q(7) = (Fh(4)*Th_t_data(4)*Heat_capacity) ;
Q(8) = (Fh(5)*Th_t_data(5)*Heat_capacity) ;

Qsk1 = Q(1) + Q(3) + Q(5);
Qsk2 = Q(2) + Q(4) + Q(6);
Qw   = Q(7) + Q(8);

Fsk1 = F(1,1) + AA(1) + F(2,1);
Fsk2 = F(1,2) + AA(2) + F(2,2);
Fw   = WW(1) + WW(2);

!Calculate Tsink based on reuse/recycle stremas;
Tout_data1 = Qsk1 /(Fsk1*Heat_capacity);
Tout_data2 = Qsk2 /(Fsk2*Heat_capacity);
Tout_w     = Qw   /(Fw*Heat_capacity);

!Overall energy balance;
@SUM(HOT(i):Cph(i)*(Th_s(i)-Th_t(i)))-@SUM(COLD(j):Cpc(j)*(Tc_t(j)-
Tc_s(j)))+ Qh - Qc = 0;

!To identify the pinch location;
@FOR(PINCH(k): @SUM(HOT(i):Cph(i)*((Lamtp(i,k)*(T_p(k)-Th_t(i)))-
Lamsp(i,k)*(T_p(k)-Th_s(i))))=A(k));

@FOR(PINCH(k):@SUM(COLD(j):Cpc(j)*((Nsp(j,k)*(T_p(k)-Tc_s(j)))-
Ntp(j,k)*(T_p(k)-Tc_t(j))))    =B(k));

@FOR(PINCH(k):A(k) - B(k) - Qc <= 0);

!Linearlisation for binary integer;
@FOR(HP(i,k):((0 - T_p(k))* Lamtp(i,k)) - (Th_t(i) - T_p(k))
<0 );

@FOR(HP(i,k):(Th_t(i) - T_p(k)) - ((1000000-T_p(k))*(1-
Lamtp(i,k)))<=0);

@FOR(HP(i,k):((0 - T_p(k))* Lamsp(i,k)) - (Th_s(i) - T_p(k))
<0);

@FOR(HP(i,k):(Th_s(i) - T_p(k)) - ((1000000-T_p(k))*(1-
Lamsp(i,k)))<=0);

@FOR(CP(j,k):((0 - T_p(k))* Ntp(j,k)) - (Tc_t(j) - T_p(k))
<0) ;

@FOR(CP(j,k):(Tc_t(j) - T_p(k)) - ((1000000-T_p(k))*(1-Ntp(j,k)))
<=0);
```

```
@FOR(CP(j,k):((0 - T_p(k))* Nsp(j,k)) - (Tc_s(j) - T_p(k))
<0);

@FOR(CP(j,k):(Tc_s(j) - T_p(k)) - ((1000000-T_p(k))*(1-Nsp(j,k)))
<=0);

!Binary integer;
@FOR(HP(i,k):@BIN(Lamtp(i,k));@BIN(Lamsp(i,k)));
@FOR(CP(j,k):@BIN(Ntp(j,k)); @BIN(Nsp(j,k)));

END
```

Appendix D2 – HIRCN solution for Case study 2

```
Global optimal solution found.
  Objective value:                              254630.8
  Objective bound:                              254630.8
  Infeasibilities:                              0.000000
  Extended solver steps:                               2
  Total solver iterations:                         64356

  Model Class:                                     MINLP

  Total variables:                    290
  Nonlinear variables:                191
  Integer variables:                  168

  Total constraints:                  438
  Nonlinear constraints:               36

  Total nonzeros:                    1053
  Nonlinear nonzeros:                 353
```

Variable	Value	Reduced Cost
CA	0.000000	0.000000
TOXA	0.000000	0.000000
THODA	0.000000	0.000000
PHA	7.000000	0.000000
DA	2.204000	0.000000
VA	1.002000	0.000000
TOUT_DATA1	151.0261	0.000000
TOUT_DATA2	110.0000	0.000000
TOUT_W	35.00000	0.000000
TOTAL_AA	3523.074	0.000000
COST_AA	72.00000	0.000000
QC	80785.84	0.000000
COST_CW	0.1200000E-01	0.000000
QH	0.000000	5.269000
COST_HH	5.269000	0.000000
TOTAL_WW	3973.074	0.000000
DT	10.00000	0.000000
HEAT_CAPACITY	1.797600	0.000000
QSK1	814453.6	0.000000
QSK2	375698.4	0.000000
QW	249969.9	0.000000
FSK1	3000.000	0.000000
FSK2	1900.000	0.000000
FW	3973.074	0.000000
TH_S(1)	155.0000	0.000000
TH_S(2)	155.0000	0.000000
TH_S(3)	115.0000	0.000000
TH_S(4)	155.0000	0.000000
TH_S(5)	115.0000	0.000000
TH_T(1)	154.0000	0.000000
TH_T(2)	105.0000	0.000000
TH_T(3)	105.0000	0.000000
TH_T(4)	30.00000	0.000000
TH_T(5)	30.00000	0.000000
CPH(1)	1272.397	0.000000
CPH(2)	1009.912	0.000000
CPH(3)	192.8527	0.000000
CPH(4)	2930.731	0.000000

```
       CPH( 5)        4211.267          0.000000
        FH( 1)        707.8311          0.000000
        FH( 2)        561.8110          0.000000
        FH( 3)        107.2834          0.000000
        FH( 4)        1630.358          0.000000
        FH( 5)        2342.717          0.000000
    COST_H( 1)        0.000000          0.000000
    COST_H( 2)        0.000000          0.000000
    COST_H( 3)        0.000000          0.000000
    COST_H( 4)        0.000000          0.000000
    COST_H( 5)        0.000000          0.000000
 TH_S_DATA( 1)        160.0000          0.000000
 TH_S_DATA( 2)        160.0000          0.000000
 TH_S_DATA( 3)        120.0000          0.000000
 TH_S_DATA( 4)        160.0000          0.000000
 TH_S_DATA( 5)        120.0000          0.000000
 TH_T_DATA( 1)        159.0000          0.000000
 TH_T_DATA( 2)        110.0000         -12.11893
 TH_T_DATA( 3)        110.0000         -2.314230
 TH_T_DATA( 4)        35.00000         -35.16874
 TH_T_DATA( 5)        35.00000         -50.53516
      TC_S( 1)        165.0000          0.000000
      TC_S( 2)        125.0000          0.000000
      TC_S( 3)        30.00000          0.000000
      TC_S( 4)        30.00000          0.000000
      TC_T( 1)        166.0000          0.000000
      TC_T( 2)        165.0000          0.000000
      TC_T( 3)        153.5637          0.000000
      TC_T( 4)        115.0000          0.000000
       CPC( 1)        0.000000         0.4920005E-06
       CPC( 2)        0.000000          23.90391
       CPC( 3)        4120.403          0.000000
       CPC( 4)        2212.676          0.000000
        FC( 1)        0.000000          0.000000
        FC( 2)        0.000000          0.000000
        FC( 3)        2292.169          0.000000
        FC( 4)        1230.906          0.000000
    COST_C( 1)        0.000000          0.000000
    COST_C( 2)        0.000000          0.000000
    COST_C( 3)        0.000000          0.000000
    COST_C( 4)        0.000000          0.000000
 TC_S_DATA( 1)        160.0000          0.000000
 TC_S_DATA( 2)        120.0000          0.000000
 TC_S_DATA( 3)        25.00000          0.000000
 TC_S_DATA( 4)        25.00000          0.000000
 TC_T_DATA( 1)        161.0000          0.000000
 TC_T_DATA( 2)        160.0000          0.000000
 TC_T_DATA( 3)        148.5637          0.000000
 TC_T_DATA( 4)        110.0000          0.000000
       T_P( 1)        155.0000          0.000000
       T_P( 2)        155.0000          0.000000
       T_P( 3)        115.0000          0.000000
       T_P( 4)        155.0000          0.000000
       T_P( 5)        115.0000          0.000000
       T_P( 6)        165.0000          0.000000
       T_P( 7)        125.0000          0.000000
       T_P( 8)        30.00000          0.000000
       T_P( 9)        30.00000          0.000000
         A( 1)        777995.6          0.000000
         A( 2)        777995.6          0.000000
         A( 3)        619097.5          0.000000
```

A(4)	777995.6	0.000000
A(5)	619097.5	0.000000
A(6)	777995.6	0.000000
A(7)	658503.9	0.000000
A(8)	0.000000	0.000000
A(9)	0.000000	0.000000
B(1)	697209.8	0.000000
B(2)	697209.8	0.000000
B(3)	538311.7	0.000000
B(4)	697209.8	0.000000
B(5)	538311.7	0.000000
B(6)	697209.8	0.000000
B(7)	579515.7	0.000000
B(8)	0.000000	0.000000
B(9)	0.000000	0.000000
LAMTP(1, 1)	1.000000	0.000000
LAMTP(1, 2)	1.000000	0.000000
LAMTP(1, 3)	0.000000	-595.4819
LAMTP(1, 4)	1.000000	0.000000
LAMTP(1, 5)	0.000000	-0.5956323E-03
LAMTP(1, 6)	1.000000	0.000000
LAMTP(1, 7)	0.000000	0.000000
LAMTP(1, 8)	0.000000	0.000000
LAMTP(1, 9)	0.000000	0.000000
LAMTP(2, 1)	1.000000	0.000000
LAMTP(2, 2)	1.000000	0.000000
LAMTP(2, 3)	1.000000	121.1894
LAMTP(2, 4)	1.000000	0.000000
LAMTP(2, 5)	1.000000	0.1212200E-03
LAMTP(2, 6)	1.000000	0.000000
LAMTP(2, 7)	1.000000	0.000000
LAMTP(2, 8)	0.000000	0.000000
LAMTP(2, 9)	0.000000	0.000000
LAMTP(3, 1)	1.000000	0.000000
LAMTP(3, 2)	1.000000	0.000000
LAMTP(3, 3)	1.000000	23.14232
LAMTP(3, 4)	1.000000	0.000000
LAMTP(3, 5)	1.000000	0.2314817E-04
LAMTP(3, 6)	1.000000	0.000000
LAMTP(3, 7)	1.000000	0.000000
LAMTP(3, 8)	0.000000	0.000000
LAMTP(3, 9)	0.000000	0.000000
LAMTP(4, 1)	1.000000	0.000000
LAMTP(4, 2)	1.000000	0.000000
LAMTP(4, 3)	1.000000	2989.346
LAMTP(4, 4)	1.000000	0.000000
LAMTP(4, 5)	1.000000	0.2990101E-02
LAMTP(4, 6)	1.000000	0.000000
LAMTP(4, 7)	1.000000	0.000000
LAMTP(4, 8)	1.000000	0.000000
LAMTP(4, 9)	1.000000	0.000000
LAMTP(5, 1)	1.000000	0.000000
LAMTP(5, 2)	1.000000	0.000000
LAMTP(5, 3)	1.000000	4295.493
LAMTP(5, 4)	1.000000	0.000000
LAMTP(5, 5)	1.000000	0.4296577E-02
LAMTP(5, 6)	1.000000	0.000000
LAMTP(5, 7)	1.000000	0.000000
LAMTP(5, 8)	1.000000	0.000000
LAMTP(5, 9)	1.000000	0.000000
LAMSP(1, 1)	0.000000	0.000000

```
LAMSP( 1, 2)        0.000000          0.000000
LAMSP( 1, 3)        0.000000          610.7507
LAMSP( 1, 4)        0.000000          0.000000
LAMSP( 1, 5)        0.000000         0.6109049E-03
LAMSP( 1, 6)        1.000000          0.000000
LAMSP( 1, 7)        0.000000          0.000000
LAMSP( 1, 8)        0.000000          0.000000
LAMSP( 1, 9)        0.000000          0.000000
LAMSP( 2, 1)        0.000000          0.000000
LAMSP( 2, 2)        0.000000          0.000000
LAMSP( 2, 3)        0.000000          484.7575
LAMSP( 2, 4)        0.000000          0.000000
LAMSP( 2, 5)        0.000000         0.4848799E-03
LAMSP( 2, 6)        1.000000          0.000000
LAMSP( 2, 7)        0.000000          0.000000
LAMSP( 2, 8)        0.000000          0.000000
LAMSP( 2, 9)        0.000000          0.000000
LAMSP( 3, 1)        1.000000          0.000000
LAMSP( 3, 2)        1.000000          0.000000
LAMSP( 3, 3)        0.000000          0.000000
LAMSP( 3, 4)        1.000000          0.000000
LAMSP( 3, 5)        0.000000          0.000000
LAMSP( 3, 6)        1.000000          0.000000
LAMSP( 3, 7)        1.000000          0.000000
LAMSP( 3, 8)        0.000000          0.000000
LAMSP( 3, 9)        0.000000          0.000000
LAMSP( 4, 1)        0.000000          0.000000
LAMSP( 4, 2)        0.000000          0.000000
LAMSP( 4, 3)        0.000000          1406.751
LAMSP( 4, 4)        0.000000          0.000000
LAMSP( 4, 5)        0.000000         0.1407106E-02
LAMSP( 4, 6)        1.000000          0.000000
LAMSP( 4, 7)        0.000000          0.000000
LAMSP( 4, 8)        0.000000          0.000000
LAMSP( 4, 9)        0.000000          0.000000
LAMSP( 5, 1)        1.000000          0.000000
LAMSP( 5, 2)        1.000000          0.000000
LAMSP( 5, 3)        0.000000          0.000000
LAMSP( 5, 4)        1.000000          0.000000
LAMSP( 5, 5)        0.000000          0.000000
LAMSP( 5, 6)        1.000000          0.000000
LAMSP( 5, 7)        1.000000          0.000000
LAMSP( 5, 8)        0.000000          0.000000
LAMSP( 5, 9)        0.000000          0.000000
  NTP( 1, 1)        0.000000          0.000000
  NTP( 1, 2)        0.000000          0.000000
  NTP( 1, 3)        0.000000          0.000000
  NTP( 1, 4)        0.000000          0.000000
  NTP( 1, 5)        0.000000          0.000000
  NTP( 1, 6)        0.000000          0.000000
  NTP( 1, 7)        0.000000          0.000000
  NTP( 1, 8)        0.000000          0.000000
  NTP( 1, 9)        0.000000          0.000000
  NTP( 2, 1)        0.000000          0.000000
  NTP( 2, 2)        0.000000          0.000000
  NTP( 2, 3)        0.000000          0.000000
  NTP( 2, 4)        0.000000          0.000000
  NTP( 2, 5)        0.000000          0.000000
  NTP( 2, 6)        0.000000          0.000000
  NTP( 2, 7)        0.000000          0.000000
  NTP( 2, 8)        0.000000          0.000000
```

NTP(2, 9)	0.000000	0.000000
NTP(3, 1)	1.000000	0.000000
NTP(3, 2)	1.000000	0.000000
NTP(3, 3)	0.000000	-1906.787
NTP(3, 4)	1.000000	0.000000
NTP(3, 5)	0.000000	-0.1907269E-02
NTP(3, 6)	1.000000	0.000000
NTP(3, 7)	0.000000	0.000000
NTP(3, 8)	0.000000	0.000000
NTP(3, 9)	0.000000	0.000000
NTP(4, 1)	1.000000	0.000000
NTP(4, 2)	1.000000	0.000000
NTP(4, 3)	0.000000	0.000000
NTP(4, 4)	1.000000	0.000000
NTP(4, 5)	1.000000	0.000000
NTP(4, 6)	1.000000	0.000000
NTP(4, 7)	1.000000	0.000000
NTP(4, 8)	0.000000	0.000000
NTP(4, 9)	0.000000	0.000000
NSP(1, 1)	0.000000	0.000000
NSP(1, 2)	0.000000	0.000000
NSP(1, 3)	0.000000	0.000000
NSP(1, 4)	0.000000	0.000000
NSP(1, 5)	0.000000	0.000000
NSP(1, 6)	0.000000	0.000000
NSP(1, 7)	0.000000	0.000000
NSP(1, 8)	0.000000	0.000000
NSP(1, 9)	0.000000	0.000000
NSP(2, 1)	1.000000	0.000000
NSP(2, 2)	1.000000	0.000000
NSP(2, 3)	0.000000	0.000000
NSP(2, 4)	1.000000	0.000000
NSP(2, 5)	0.000000	0.000000
NSP(2, 6)	1.000000	0.000000
NSP(2, 7)	0.000000	0.000000
NSP(2, 8)	0.000000	0.000000
NSP(2, 9)	0.000000	0.000000
NSP(3, 1)	1.000000	0.000000
NSP(3, 2)	1.000000	0.000000
NSP(3, 3)	1.000000	-4202.811
NSP(3, 4)	1.000000	0.000000
NSP(3, 5)	1.000000	-0.4203872E-02
NSP(3, 6)	1.000000	0.000000
NSP(3, 7)	1.000000	0.000000
NSP(3, 8)	0.000000	0.000000
NSP(3, 9)	0.000000	0.000000
NSP(4, 1)	1.000000	0.000000
NSP(4, 2)	1.000000	0.000000
NSP(4, 3)	1.000000	-2256.929
NSP(4, 4)	1.000000	0.000000
NSP(4, 5)	1.000000	-0.2257499E-02
NSP(4, 6)	1.000000	0.000000
NSP(4, 7)	1.000000	0.000000
NSP(4, 8)	0.000000	0.000000
NSP(4, 9)	0.000000	0.000000
H(1)	0.000000	0.000000
H(2)	0.000000	0.000000
H(3)	0.000000	0.000000
H(4)	0.000000	0.000000
H(5)	0.000000	0.000000
H(6)	0.000000	0.000000

```
        FR( 1)        2900.000             0.000000
        FR( 2)        2450.000             0.000000
        CR( 1)      0.3300000E-01          0.000000
        CR( 2)      0.2200000E-01          0.000000
        WW( 1)        1630.358             0.000000
        WW( 2)        2342.717             0.000000
      TOXR( 1)      0.8000000              0.000000
      TOXR( 2)      0.5000000              0.000000
     THODR( 1)       75.00000              0.000000
     THODR( 2)       88.00000              0.000000
       PHR( 1)       5.300000              0.000000
       PHR( 2)       5.100000              0.000000
        DR( 1)       2.000000              0.000000
        DR( 2)       2.208000              0.000000
        VR( 1)       1.256000              0.000000
        VR( 2)       1.220000              0.000000
        FK( 1)        3000.000             0.000000
        FK( 2)        1900.000             0.000000
        CK( 1)      0.1300000E-01          0.000000
        CK( 2)      0.1100000E-01          0.000000
        AA( 1)        2292.169             0.000000
        AA( 2)        1230.906             0.000000
      TOXK( 1)       2.000000              0.000000
      TOXK( 2)       2.000000              0.000000
     THODK( 1)       75.00000              0.000000
     THODK( 2)       75.00000              0.000000
       PHK( 1)       5.900000              0.000000
       PHK( 2)       5.700000              0.000000
        DK( 1)       1.893848              0.000000
        DK( 2)       2.119296              0.000000
        VK( 1)       1.056864              0.000000
        VK( 2)       1.083200              0.000000
      F( 1, 1)       707.8311              0.000000
      F( 1, 2)       561.8110              0.000000
      F( 2, 1)       0.000000              0.000000
      F( 2, 2)       107.2834              0.000000
        TS( 1)       0.000000              0.000000
        TS( 2)       0.000000              0.000000
        TS( 3)       0.000000              0.000000
        TS( 4)       0.000000              0.000000
        TS( 5)       0.000000              0.000000
        TS( 6)       0.000000              0.000000
        TS( 7)       0.000000              0.000000
        TS( 8)       0.000000              0.000000
        TS( 9)       0.000000              0.000000
        TT( 1)       0.000000              0.000000
        TT( 2)       0.000000              0.000000
        TT( 3)       0.000000              0.000000
        TT( 4)       0.000000              0.000000
        TT( 5)       0.000000              0.000000
        TT( 6)       0.000000              0.000000
        TT( 7)       0.000000              0.000000
        TT( 8)       0.000000              0.000000
        TT( 9)       0.000000              0.000000
         Q( 1)       202311.2              0.000000
         Q( 2)       111090.3              0.000000
         Q( 3)       612142.4              0.000000
         Q( 4)       243394.3              0.000000
         Q( 5)       0.000000              0.000000
         Q( 6)       21213.80              0.000000
         Q( 7)       102575.6              0.000000
```

```
Q( 8)        147394.4          0.000000
```

APPENDIX E: HIRCN with heat of mixing mathematical model and solution for Case study 3 in Chapter 6

Appendix E1 – HIRCN with heat of mixing mathematical model for Case study 3

```
!Final coding after discretisation;

SETS:

SOURCES/1..4/      : C_R, F_R, T_R, FR_Cp;

JUNCTIONS_A/1..8/  : C_A, F_A, T_A, U, FA_Cp, Q_A, H_mixing_A,
                     FA_kg_acetone, FA_kgmol_acetone, FA_kg_water,
                     FA_kgmol_water, FA_x_acetone, FA_x_water,
                     G12_A, G21_A, Tau12_A, Tau21_A, moleA;
JUNCTIONS_D/1..8/  : C_D, F_D, T_D, FD_Cp;

SINKS/1..4/        : CK_in, F_K, TK_in, FK_Cp, H_mixing,
                     FK_kg_acetone, FK_kgmol_acetone, FK_kg_water,
                     FK_kgmol_water, FK_x_acetone, FK_x_water,
                     G12, G21, Tau12, Tau21, molesink;

STREAMS_RA(SOURCES, JUNCTIONS_A)          : F_RA;

STREAMS_DK(JUNCTIONS_D, SINKS)            : F_DK;

BYPASS_1(SOURCES, SINKS)                  : B_RK;

HEN_1/1..4/        : T_AH_IN, T_AH_OUT, T_AC_IN, T_AC_OUT, MCPH_A,
                     MCPC_A;

PINCH_1/1..8/      : TP_A, A, B;

PINCH_BIN(HEN_1, PINCH_1): LAMSP, LAMTP, NSP, NTP;

ENDSETS

DATA:

T_A = 75 100 20 20 75 100 75 24;
T_D = 30 30 100 70 30 30 100 65;

ENDDATA

@BND(790, C_A(1), 800);
@BND(1090, C_A(2),1100);
C_A(3)  = 0;
C_A(4)  = 0;
@BND(790, C_A(5), 800);
@BND(1090, C_A(6),1100);
@BND(790, C_A(7), 800);
@BND(45, C_A(8),50);
```

```
!Data Input;
F_R(1) = 100;
F_R(2) = 40;
F_R(3) = 166.67;
C_R(1) = 100;
C_R(2) = 800;
C_R(3) = 1100;
C_R(4) = 0;
T_R(1) = 100;
T_R(2) = 75;
T_R(3) = 100;
T_R(4) = 20;

F_K(1) = 100;
F_K(2) = 40;
F_K(3) = 166.67;
CK_in(1) = 50;
CK_in(2) = 50;
CK_in(3) = 800;
TK_in(1) = 100;
TK_in(2) = 75;
TK_in(3) = 100;
TK_in(4) = 30;

!molecular weight of acetone and water;
MW_acetone = 58.08;     !kg/kmol;
MW_water  = 18;         !kg/kmol;

!Objective Functions;
MIN = F_R(4)*Cost_AA + QC*Cost_CW + QH*Cost_HH;
Cost_AA = 12960; !$/yr;
Cost_CW = 20; !$/yr;
Cost_HH = 80;!$/yr;

!Mass Balance around sources;
@FOR (SOURCES(i):
      @SUM(JUNCTIONS_A(j):F_RA(i, j)) + @SUM(SINKS(l):B_RK(i, l)) =
      F_R(i));

!Mass Balance around junctions_A;
@FOR (JUNCTIONS_A(j):
      @SUM(SOURCES(i):F_RA(i, j)) = F_A(j));

!Composition Balance around junctions_A;
@FOR (JUNCTIONS_A(j):
      @SUM(SOURCES(i):F_RA(i, j)*C_R(i)) = F_A(j)*C_A(j));

!Energy Balance around junctions_A;
@FOR (JUNCTIONS_A(j):
      @SUM(SOURCES(i):F_RA(i, j)*T_R(i)*4.2) + H_mixing_A(j) =
      F_A(j)*T_A(j)*4.2);

!Mass Balance around junctions_D;
@FOR (JUNCTIONS_D(k):
      @SUM(SINKS(l):F_DK(k, l)) = F_D(k));

!Mass Balance around sinks;
@FOR (SINKS(l):
      @SUM(JUNCTIONS_D(k):F_DK(k, l)) + @SUM(SOURCES(i):B_RK(i, l))
      = F_K(l));
```

```
!Composition Balance around sinks;
@FOR (SINKS(l):
      @SUM(JUNCTIONS_D(k):F_DK(k, l)*C_D(k)) +
      @SUM(SOURCES(i):B_RK(i, l)*C_R(i)) <= F_K(l)*CK_in(l));

!Energy Balance around sinks;
@FOR (SINKS(l):
      @SUM(JUNCTIONS_D(k):F_DK(k, l)*T_D(k)*4.2) +
      @SUM(SOURCES(i):B_RK(i, l)*T_R(i)*4.2) + H_mixing(l) =
      F_K(l)*TK_in(l)*4.2);

!Cp calculation for junction A;
@FOR(JUNCTIONS_A(j):FA_kg_acetone(j) = 100 * C_A(j)/1000000);
@FOR(JUNCTIONS_A(j):FA_kg_water(j)  = 100 - FA_kg_acetone(j));
@FOR(JUNCTIONS_A(j):FA_kgmol_acetone(j) = FA_kg_acetone(j)/
MW_acetone);
@FOR(JUNCTIONS_A(j):FA_kgmol_water(j)  = FA_kg_water(j) / MW_water);
@FOR(JUNCTIONS_A(j):FA_x_acetone(j) = FA_kgmol_acetone(j) /
(FA_kgmol_water(j) + FA_kgmol_acetone(j)));
@FOR(JUNCTIONS_A(j):FA_x_water(j)  = FA_kgmol_water(j)  /
(FA_kgmol_water(j) + FA_kgmol_acetone(j)));
@FOR(JUNCTIONS_A(j):FA_x_acetone(j) <=1);
@FOR(JUNCTIONS_A(j):FA_x_water(j)  <=1);

!Heat of mixing calculation at junctions_A;
@FOR(JUNCTIONS_A(j):H_mixing_A(j) = 8.314 *
FA_x_acetone(j)*FA_x_water(j)*moleA(j)*T_A(j)*
((G21_A(j)*Tau21_A(j))/(FA_x_acetone(j) + FA_x_water(j) *G21_A(j)) +
(G12_A(j)*Tau12_A(j))/(FA_x_water(j)  + FA_x_acetone(j)*G12_A(j))));

@FOR(JUNCTIONS_A(j):moleA(j) = (F_A(j)*C_A(j)/1000000)/MW_acetone +
(F_A(j)*(1-(C_A(j)/1000000)))/MW_water);

@FOR(JUNCTIONS_A(j):G12_A(j) = @EXP(-0.5343*Tau12_A(j)));

@FOR(JUNCTIONS_A(j):G21_A(j) = @EXP(-0.5343*Tau21_A(j)));

@FOR(JUNCTIONS_A(j):Tau12_A(j) = (631.05/(8.314*(T_A(j) +
273.15))));

@FOR(JUNCTIONS_A(j):Tau21_A(j) = (1197.41/(8.314*(T_A(j) +
273.15))));

@FOR(JUNCTIONS_A(j):@FREE(G12_A);

@FREE(G21_A);@FREE(Tau12_A);@FREE(Tau21_A); @FREE(H_mixing_A));

!Mass fraction (x1, x2) for process sinks;
@FOR(SINKS(l):FK_kg_acetone(l) = 100*CK_in(l)/1000000);

@FOR(SINKS(l):FK_kg_water(l)  = 100 - FK_kg_acetone(l));

@FOR(SINKS(l):FK_kgmol_acetone(l) = FK_kg_acetone(l)/ MW_acetone);

@FOR(SINKS(l):FK_kgmol_water(l)  = FK_kg_water(l) / MW_water);

@FOR(SINKS(l):FK_x_acetone(l) = FK_kgmol_acetone(l) /
(FK_kgmol_water(l) + FK_kgmol_acetone(l)));

@FOR(SINKS(l):FK_x_water(l)  = FK_kgmol_water(l)  /
(FK_kgmol_water(l) + FK_kgmol_acetone(l)));
```

```
@FOR(SINKS(l):FK_x_acetone(l) <=1);

@FOR(SINKS(l):FK_x_water(l)  <=1);

!Heat of mixing calculation at sink;
@FOR(SINKS(l):H_mixing(l) =   8.314 *
FK_x_acetone(l)*FK_x_water(l)*molesink(l)*TK_in(l)*
(G21(l)*Tau21(l))/(FK_x_acetone(l) + FK_x_water(l) *G21(l)) +
(G12(l)*Tau12(l))/(FK_x_water(l)  + FK_x_acetone(l)*G12(l))));

@FOR(SINKS(l):molesink(l) = (F_K(l)*CK_in(l)/1000000)/MW_acetone +
(F_K(l)*(1-(CK_in(l)/1000000)))/MW_water);

@FOR(SINKS(l):G12(l) = @EXP(-0.5343*Tau12(l)));

@FOR(SINKS(l):G21(l) = @EXP(-0.5343*Tau21(l)));

@FOR(SINKS(l):Tau12(l) = (631.05/(8.314*(TK_in(l) + 273.15))));

@FOR(SINKS(l):Tau21(l) = (1197.41/(8.314*(TK_in(l) + 273.15))));

@FOR(SINKS(l):@FREE(G12);@FREE(G21); @FREE(Tau12); @FREE(Tau21);
@FREE(H_mixing));

!No fresh got to waste;
B_RK(4, 4) = 0;

!Flowrate and concentration at JUNCTIONS_A is the same at
JUNCTIONS_D;
C_A(1)  = C_D(1);
C_A(2)  = C_D(2);
C_A(3)  = C_D(3);
C_A(4)  = C_D(4);
C_A(5)  = C_D(5);
C_A(6)  = C_D(6);
C_A(7)  = C_D(7);
C_A(8)  = C_D(8);

F_A(1) = F_D(1);
F_A(2) = F_D(2);
F_A(3) = F_D(3);
F_A(4) = F_D(4);
F_A(5) = F_D(5);
F_A(6) = F_D(6);
F_A(7) = F_D(7);
F_A(8) = F_D(8);

!Set the maximum of F_A;
@FOR(JUNCTIONS_A(j): F_A(j) <= 306.67*U(j));

!Only have 4 junctions;
@SUM(JUNCTIONS_A(j): U(j)) = 8;

!U(j) is binary variable;
@FOR(JUNCTIONS_A(j): @BIN (U(j)));

!Constant values;
DT = 10;
CP = 4.2; !Unit = kJ/kg.K;
```

```
!Identifying (shifted temperatures) hot and cold streams;
 T_AH_IN(1)*2  = T_A(1)*2 - DT;
T_AH_OUT(1)*2  = T_D(1)*2 - DT;
 T_AH_IN(2)*2  = T_A(2)*2 - DT;
T_AH_OUT(2)*2  = T_D(2)*2 - DT;

 T_AC_IN(1)*2  = T_A(3)*2 + DT;
T_AC_OUT(1)*2  = T_D(3)*2 + DT;
 T_AC_IN(2)*2  = T_A(4)*2 + DT;
T_AC_OUT(2)*2  = T_D(4)*2 + DT;

 T_AH_IN(3)*2  = T_A(5)*2 - DT;
T_AH_OUT(3)*2  = T_D(5)*2 - DT;
 T_AH_IN(4)*2  = T_A(6)*2 - DT;
T_AH_OUT(4)*2  = T_D(6)*2 - DT;

 T_AC_IN(3)*2  = T_A(7)*2 + DT;
T_AC_OUT(3)*2  = T_D(7)*2 + DT;
 T_AC_IN(4)*2  = T_A(8)*2 + DT;
T_AC_OUT(4)*2  = T_D(8)*2 + DT;

!MCP values;
MCPH_A(1) = CP*F_A(1);
MCPH_A(2) = CP*F_A(2);
MCPC_A(1) = CP*F_A(3);
MCPC_A(2) = CP*F_A(4);

MCPH_A(3) = CP*F_A(5);
MCPH_A(4) = CP*F_A(6);
MCPC_A(3) = CP*F_A(7);
MCPC_A(4) = CP*F_A(8);

!Assigning pinch temperatures = supply temperatures;
TP_A(1) = T_AH_IN(1);
TP_A(2) = T_AH_IN(2);
TP_A(3) = T_AC_IN(1);
TP_A(4) = T_AC_IN(2);

TP_A(5) = T_AH_IN(3);
TP_A(6) = T_AH_IN(4);
TP_A(7) = T_AC_IN(3);
TP_A(8) = T_AC_IN(4);

!Identifying pinch location (BIN=1 below pinch, BIN=0, above pinch);
@FOR (PINCH_BIN(m, n):
      (0-TP_A(n))*LAMSP(m, n) < T_AH_IN(m)-TP_A(n);
      (10e6-TP_A(n))*(1-LAMSP(m, n)) >= T_AH_IN(m)-TP_A(n);

      (0-TP_A(n))*LAMTP(m, n) < T_AH_OUT(m)-TP_A(n);
      (10e6-TP_A(n))*(1-LAMTP(m, n)) >= T_AH_OUT(m)-TP_A(n);

      (0-TP_A(n))*NSP(m, n) < T_AC_IN(m)-TP_A(n);
      (10e6-TP_A(n))*(1-NSP(m, n)) >= T_AC_IN(m)-TP_A(n);

      (0-TP_A(n))*NTP(m, n) < T_AC_OUT(m)-TP_A(n);
      (10e6-TP_A(n))*(1-NTP(m, n)) >= T_AC_OUT(m)-TP_A(n));

@FOR (PINCH_1(n):
      @SUM(HEN_1(m):MCPH_A(m)*(LAMTP(m, n)*(TP_A(n)-T_AH_OUT(m))-
      LAMSP(m, n)*(TP_A(n)-T_AH_IN(m)))) = A(n);
```

```
    @SUM(HEN_1(o):MCPC_A(o)*(NSP(o, n)*(TP_A(n)-T_AC_IN(o))-NTP(o,
    n)*(TP_A(n)-T_AC_OUT(o)))) = B(n);

    A(n) - B(n) <= QC);

!Overall energy balance;
@SUM(HEN_1(m):MCPH_A(m)*(T_AH_IN(m)-T_AH_OUT(m))) -
@SUM(HEN_1(m):MCPC_A(m)*(T_AC_OUT(m)-T_AC_IN(m))) + QH - QC = 0;

!Defining binary integers;
@FOR (PINCH_BIN(m, n):@BIN(LAMTP(m,n)); @BIN(LAMSP(m,n));
@BIN (NTP(m,n)); @BIN(NSP(m,n)));

!Defining integer variables;
@FOR (SOURCES(i):@GIN(T_R(i)));
@FOR (SINKS(l): @GIN(TK_in(l)));
@FOR (JUNCTIONS_A(j):@GIN(T_A(j)));
@FOR (JUNCTIONS_D(k):@GIN(T_D(k)));
@FOR (HEN_1(m): @GIN(T_AH_IN(m)); @GIN(T_AH_OUT(m));
@GIN (T_AC_IN(m)); @GIN(T_AC_OUT(m)); @GIN(TP_A(m)));

End
```

Appendix E2 – HIRCN with heat of mixing mathematical model for Case study 3

```
Global optimal solution found.
  Objective value:                              1542245.
  Objective bound:                              1542245.
  Infeasibilities:                              0.000000
  Extended solver steps:                              75
  Total solver iterations:                       4219242

  Model Class:                                     MINLP

  Total variables:                    364
  Nonlinear variables:                191
  Integer variables:                  136

  Total constraints:                  445
  Nonlinear constraints:               54

  Total nonzeros:                    1083
  Nonlinear nonzeros:                 293

                Variable           Value        Reduced Cost
              MW_ACETONE        58.08000            0.000000
                MW_WATER        18.00000            0.000000
                 COST_AA        12960.00            0.000000
                      QC        2812.721            0.000000
                 COST_CW        20.00000            0.000000
                      QH        6056.257            0.000000
                 COST_HH        80.00000            0.000000
                      DT        10.00000            0.000000
                      CP        4.200000            0.000000
                 C_R( 1)        100.0000            0.000000
                 C_R( 2)        800.0000            0.000000
                 C_R( 3)        1100.000            0.000000
                 C_R( 4)        0.000000            0.000000
                 F_R( 1)        100.0000            0.000000
                 F_R( 2)        40.00000            0.000000
                 F_R( 3)        166.6700            0.000000
                 F_R( 4)        77.27543            0.000000
                 T_R( 1)        100.0000            0.000000
                 T_R( 2)        75.00000            0.000000
                 T_R( 3)        100.0000            0.000000
                 T_R( 4)        20.00000            0.000000
               FR_CP( 1)        0.000000            0.000000
               FR_CP( 2)        0.000000            0.000000
               FR_CP( 3)        0.000000            0.000000
               FR_CP( 4)        0.000000            0.000000
                 C_A( 1)        790.0000            0.000000
                 C_A( 2)        1099.974            0.000000
                 C_A( 3)        0.000000            0.000000
                 C_A( 4)        0.000000            0.000000
                 C_A( 5)        790.0000            0.000000
                 C_A( 6)        1099.974            0.000000
                 C_A( 7)        799.9819            0.000000
                 C_A( 8)        50.00000        -0.8385826E-08
                 F_A( 1)        0.000000            0.000000
                 F_A( 2)        77.27543            0.000000
                 F_A( 3)        65.09915            0.000000
                 F_A( 4)        0.000000            0.000000
                 F_A( 5)        0.000000            0.000000
```

F_A(6)	0.000000	0.000000
F_A(7)	38.94474	0.000000
F_A(8)	0.000000	0.000000
T_A(1)	75.00000	0.000000
T_A(2)	100.0000	0.000000
T_A(3)	20.00000	0.000000
T_A(4)	20.00000	0.000000
T_A(5)	75.00000	0.000000
T_A(6)	100.0000	0.000000
T_A(7)	75.00000	0.000000
T_A(8)	24.00000	0.000000
U(1)	0.000000	0.000000
U(2)	1.000000	0.000000
U(3)	1.000000	0.000000
U(4)	0.000000	-2012521.
U(5)	0.000000	0.000000
U(6)	0.000000	0.000000
U(7)	1.000000	0.000000
U(8)	0.000000	-1650268.
FA_CP(1)	0.000000	0.000000
FA_CP(2)	0.000000	0.000000
FA_CP(3)	0.000000	0.000000
FA_CP(4)	0.000000	0.000000
FA_CP(5)	0.000000	0.000000
FA_CP(6)	0.000000	0.000000
FA_CP(7)	0.000000	0.000000
FA_CP(8)	0.000000	0.000000
Q_A(1)	0.000000	0.000000
Q_A(2)	0.000000	0.000000
Q_A(3)	0.000000	0.000000
Q_A(4)	0.000000	0.000000
Q_A(5)	0.000000	0.000000
Q_A(6)	0.000000	0.000000
Q_A(7)	0.000000	0.000000
Q_A(8)	0.000000	0.000000
H_MIXING_A(1)	0.000000	0.000000
H_MIXING_A(2)	0.6913791	0.000000
H_MIXING_A(3)	0.000000	0.000000
H_MIXING_A(4)	0.000000	0.000000
H_MIXING_A(5)	0.000000	0.000000
H_MIXING_A(6)	0.000000	0.000000
H_MIXING_A(7)	0.2032164	0.000000
H_MIXING_A(8)	0.000000	0.000000
FA_KG_ACETONE(1)	0.7900000E-01	0.000000
FA_KG_ACETONE(2)	0.1099974	0.000000
FA_KG_ACETONE(3)	0.000000	0.000000
FA_KG_ACETONE(4)	0.000000	0.000000
FA_KG_ACETONE(5)	0.7900000E-01	0.000000
FA_KG_ACETONE(6)	0.1099974	0.000000
FA_KG_ACETONE(7)	0.7999819E-01	0.000000
FA_KG_ACETONE(8)	0.5000000E-02	0.000000
FA_KGMOL_ACETONE(1)	0.1360193E-02	0.000000
FA_KGMOL_ACETONE(2)	0.1893895E-02	0.000000
FA_KGMOL_ACETONE(3)	0.000000	0.000000
FA_KGMOL_ACETONE(4)	0.000000	0.000000
FA_KGMOL_ACETONE(5)	0.1360193E-02	0.000000
FA_KGMOL_ACETONE(6)	0.1893895E-02	0.000000
FA_KGMOL_ACETONE(7)	0.1377379E-02	0.000000
FA_KGMOL_ACETONE(8)	0.8608815E-04	0.000000
FA_KG_WATER(1)	99.92100	0.000000
FA_KG_WATER(2)	99.89000	0.000000

FA_KG_WATER(3)	100.0000	0.000000
FA_KG_WATER(4)	100.0000	0.000000
FA_KG_WATER(5)	99.92100	0.000000
FA_KG_WATER(6)	99.89000	0.000000
FA_KG_WATER(7)	99.92000	0.000000
FA_KG_WATER(8)	99.99500	0.000000
FA_KGMOL_WATER(1)	5.551167	0.000000
FA_KGMOL_WATER(2)	5.549445	0.000000
FA_KGMOL_WATER(3)	5.555556	0.000000
FA_KGMOL_WATER(4)	5.555556	0.000000
FA_KGMOL_WATER(5)	5.551167	0.000000
FA_KGMOL_WATER(6)	5.549445	0.000000
FA_KGMOL_WATER(7)	5.551111	0.000000
FA_KGMOL_WATER(8)	5.555278	0.000000
FA_X_ACETONE(1)	0.2449683E-03	0.000000
FA_X_ACETONE(2)	0.3411601E-03	0.000000
FA_X_ACETONE(3)	0.000000	0.000000
FA_X_ACETONE(4)	0.000000	0.000000
FA_X_ACETONE(5)	0.2449683E-03	0.000000
FA_X_ACETONE(6)	0.3411601E-03	0.000000
FA_X_ACETONE(7)	0.2480652E-03	0.000000
FA_X_ACETONE(8)	0.1549640E-04	0.000000
FA_X_WATER(1)	0.9997550	0.000000
FA_X_WATER(2)	0.9996588	0.000000
FA_X_WATER(3)	1.000000	0.000000
FA_X_WATER(4)	1.000000	0.000000
FA_X_WATER(5)	0.9997550	0.000000
FA_X_WATER(6)	0.9996588	0.000000
FA_X_WATER(7)	0.9997519	0.000000
FA_X_WATER(8)	0.9999845	0.000000
G12_A(1)	0.8900428	0.000000
G12_A(2)	0.8970161	0.000000
G12_A(3)	0.8708022	0.000000
G12_A(4)	0.8708022	0.000000
G12_A(5)	0.8900428	0.000000
G12_A(6)	0.8970161	0.000000
G12_A(7)	0.8900428	0.000000
G12_A(8)	0.8724254	0.000000
G21_A(1)	0.8016925	0.000000
G21_A(2)	0.8136526	0.000000
G21_A(3)	0.7691269	0.000000
G21_A(4)	0.7691269	0.000000
G21_A(5)	0.8016925	0.000000
G21_A(6)	0.8136526	0.000000
G21_A(7)	0.8016925	0.000000
G21_A(8)	0.7718495	0.000000
TAU12_A(1)	0.2180155	0.000000
TAU12_A(2)	0.2034091	0.000000
TAU12_A(3)	0.2589190	0.000000
TAU12_A(4)	0.2589190	0.000000
TAU12_A(5)	0.2180155	0.000000
TAU12_A(6)	0.2034091	0.000000
TAU12_A(7)	0.2180155	0.000000
TAU12_A(8)	0.2554336	0.000000
TAU21_A(1)	0.4136818	0.000000
TAU21_A(2)	0.3859663	0.000000
TAU21_A(3)	0.4912957	0.000000
TAU21_A(4)	0.4912957	0.000000
TAU21_A(5)	0.4136818	0.000000
TAU21_A(6)	0.3859663	0.000000
TAU21_A(7)	0.4136818	0.000000

```
   TAU21_A( 8)        0.4846823              0.000000
     MOLEA( 1)         0.000000              0.000000
     MOLEA( 2)         4.289821              0.000000
     MOLEA( 3)         3.616619              0.000000
     MOLEA( 4)         0.000000              0.000000
     MOLEA( 5)         0.000000              0.000000
     MOLEA( 6)         0.000000              0.000000
     MOLEA( 7)         2.162402              0.000000
     MOLEA( 8)         0.000000              0.000000
       C_D( 1)         790.0000              0.000000
       C_D( 2)         1099.974              0.000000
       C_D( 3)         0.000000              0.000000
       C_D( 4)         0.000000              0.000000
       C_D( 5)         790.0000              0.000000
       C_D( 6)         1099.974              0.000000
       C_D( 7)         799.9819              0.000000
       C_D( 8)         50.00000              0.000000
       F_D( 1)         0.000000              0.000000
       F_D( 2)         77.27543              0.000000
       F_D( 3)         65.09915              0.000000
       F_D( 4)         0.000000              0.000000
       F_D( 5)         0.000000              0.000000
       F_D( 6)         0.000000              0.000000
       F_D( 7)         38.94474              0.000000
       F_D( 8)         0.000000              0.000000
       T_D( 1)         30.00000              0.000000
       T_D( 2)         30.00000              0.000000
       T_D( 3)         100.0000              0.000000
       T_D( 4)         70.00000              0.000000
       T_D( 5)         30.00000              0.000000
       T_D( 6)         30.00000              0.000000
       T_D( 7)         100.0000              0.000000
       T_D( 8)         65.00000              0.000000
     FD_CP( 1)         0.000000              0.000000
     FD_CP( 2)         0.000000              0.000000
     FD_CP( 3)         0.000000              0.000000
     FD_CP( 4)         0.000000              0.000000
     FD_CP( 5)         0.000000              0.000000
     FD_CP( 6)         0.000000              0.000000
     FD_CP( 7)         0.000000              0.000000
     FD_CP( 8)         0.000000              0.000000
     CK_IN( 1)         50.00000              0.000000
     CK_IN( 2)         50.00000              0.000000
     CK_IN( 3)         800.0000              0.000000
     CK_IN( 4)         1000000.              0.000000
       F_K( 1)         100.0000              0.000000
       F_K( 2)         40.00000              0.000000
       F_K( 3)         166.6700              0.000000
       F_K( 4)         77.27543              0.000000
     TK_IN( 1)         100.0000              0.000000
     TK_IN( 2)         75.00000              0.000000
     TK_IN( 3)         100.0000              0.000000
     TK_IN( 4)         30.00000              0.000000
     FK_CP( 1)         0.000000              0.000000
     FK_CP( 2)         0.000000              0.000000
     FK_CP( 3)         0.000000              0.000000
     FK_CP( 4)         0.000000              0.000000
  H_MIXING( 1)        0.4068375E-01          0.000000
  H_MIXING( 2)        0.1304891E-01          0.000000
  H_MIXING( 3)         1.084638              0.000000
  H_MIXING( 4)         0.000000              0.000000
```

FK_KG_ACETONE(1)	0.5000000E-02	0.000000
FK_KG_ACETONE(2)	0.5000000E-02	0.000000
FK_KG_ACETONE(3)	0.8000000E-01	0.000000
FK_KG_ACETONE(4)	100.0000	0.000000
FK_KGMOL_ACETONE(1)	0.8608815E-04	0.000000
FK_KGMOL_ACETONE(2)	0.8608815E-04	0.000000
FK_KGMOL_ACETONE(3)	0.1377410E-02	0.000000
FK_KGMOL_ACETONE(4)	1.721763	0.000000
FK_KG_WATER(1)	99.99500	0.000000
FK_KG_WATER(2)	99.99500	0.000000
FK_KG_WATER(3)	99.92000	0.000000
K_KG_WATER(4)	0.000000	133.6125
FK_KGMOL_WATER(1)	5.555278	0.000000
FK_KGMOL_WATER(2)	5.555278	0.000000
FK_KGMOL_WATER(3)	5.551111	0.000000
FK_KGMOL_WATER(4)	0.000000	0.000000
FK_X_ACETONE(1)	0.1549640E-04	0.000000
FK_X_ACETONE(2)	0.1549640E-04	0.000000
FK_X_ACETONE(3)	0.2480708E-03	0.000000
FK_X_ACETONE(4)	1.000000	0.000000
FK_X_WATER(1)	0.9999845	0.000000
FK_X_WATER(2)	0.9999845	0.000000
FK_X_WATER(3)	0.9997519	0.000000
FK_X_WATER(4)	0.000000	0.000000
G12(1)	0.8970161	0.000000
G12(2)	0.8900428	0.000000
G12(3)	0.8970161	0.000000
G12(4)	0.8747851	0.000000
G21(1)	0.8136526	0.000000
G21(2)	0.8016925	0.000000
G21(3)	0.8136526	0.000000
G21(4)	0.7758157	0.000000
TAU12(1)	0.2034091	0.000000
TAU12(2)	0.2180155	0.000000
TAU12(3)	0.2034091	0.000000
TAU12(4)	0.2503780	0.000000
TAU21(1)	0.3859663	0.000000
TAU21(2)	0.4136818	0.000000
TAU21(3)	0.3859663	0.000000
TAU21(4)	0.4750893	0.000000
MOLESINK(1)	5.555364	0.000000
MOLESINK(2)	2.222146	0.000000
MOLESINK(3)	9.254333	0.000000
MOLESINK(4)	1.330500	0.000000
F_RA(1, 1)	0.000000	0.000000
F_RA(1, 2)	0.000000	13898.82
F_RA(1, 3)	0.000000	0.000000
F_RA(1, 4)	0.000000	0.000000
F_RA(1, 5)	0.000000	0.000000
F_RA(1, 6)	0.000000	0.000000
F_RA(1, 7)	0.000000	10968.76
F_RA(1, 8)	0.000000	0.000000
F_RA(2, 1)	0.000000	0.000000
F_RA(2, 2)	0.6584562E-02	0.000000
F_RA(2, 3)	0.000000	351438.8
F_RA(2, 4)	0.000000	0.000000
F_RA(2, 5)	0.000000	0.000000
F_RA(2, 6)	0.000000	0.000000
F_RA(2, 7)	38.94386	0.000000
F_RA(2, 8)	0.000000	0.000000
F_RA(3, 1)	0.000000	10312.67

F_RA(3, 2)	77.26885	0.000000
F_RA(3, 3)	0.000000	490912.8
F_RA(3, 4)	0.000000	10312.67
F_RA(3, 5)	0.000000	10312.67
F_RA(3, 6)	0.000000	0.2310310E-01
F_RA(3, 7)	0.000000	10968.92
F_RA(3, 8)	0.000000	10312.67
F_RA(4, 1)	0.000000	0.000000
F_RA(4, 2)	0.000000	26077.49
F_RA(4, 3)	65.09915	0.000000
F_RA(4, 4)	0.000000	0.000000
F_RA(4, 5)	0.000000	0.000000
F_RA(4, 6)	0.000000	24131.60
F_RA(4, 7)	0.8797245E-03	0.000000
F_RA(4, 8)	0.000000	0.000000
F_DK(1, 1)	0.000000	5906.186
F_DK(1, 2)	0.000000	5906.186
F_DK(1, 3)	0.000000	19003.28
F_DK(1, 4)	0.000000	211.8670
F_DK(2, 1)	0.000000	13199.16
F_DK(2, 2)	0.000000	13199.16
F_DK(2, 3)	0.000000	23099.59
F_DK(2, 4)	77.27543	0.000000
F_DK(3, 1)	49.99988	0.000000
F_DK(3, 2)	15.09927	0.000000
F_DK(3, 3)	0.000000	1031.267
F_DK(3, 4)	0.000000	22666.95
F_DK(4, 1)	0.000000	0.000000
F_DK(4, 2)	0.000000	0.000000
_DK(4, 3)	0.000000	9693.912
F_DK(4, 4)	0.000000	18709.33
F_DK(5, 1)	0.000000	5906.186
F_DK(5, 2)	0.000000	5906.186
F_DK(5, 3)	0.000000	19003.28
F_DK(5, 4)	0.000000	211.8670
F_DK(6, 1)	0.000000	13199.16
F_DK(6, 2)	0.000000	13199.16
F_DK(6, 3)	0.000000	23099.59
F_DK(6, 4)	0.000000	0.000000
F_DK(7, 1)	0.000000	7218.684
F_DK(7, 2)	0.000000	7218.684
F_DK(7, 3)	38.94474	0.000000
F_DK(7, 4)	0.000000	10517.14
F_DK(8, 1)	0.000000	0.000000
F_DK(8, 2)	0.000000	0.000000
F_DK(8, 3)	0.000000	10622.05
F_DK(8, 4)	0.000000	16839.16
B_RK(1, 1)	50.00000	0.000000
B_RK(1, 2)	11.68623	0.000000
B_RK(1, 3)	38.31377	0.000000
B_RK(1, 4)	0.000000	20245.83
B_RK(2, 1)	0.000000	0.000000
B_RK(2, 2)	1.039222	0.000000
B_RK(2, 3)	0.1032989E-01	0.000000
B_RK(2, 4)	0.000000	0.000000
B_RK(3, 1)	0.000000	10312.67
B_RK(3, 2)	0.000000	10312.67
B_RK(3, 3)	89.40115	0.000000
B_RK(3, 4)	0.000000	6347.341
B_RK(4, 1)	0.1210826E-03	0.000000
B_RK(4, 2)	12.17528	0.000000

B_RK(4, 3)	0.000000	24131.65
B_RK(4, 4)	0.000000	0.000000
T_AH_IN(1)	70.00000	0.000000
T_AH_IN(2)	95.00000	0.000000
T_AH_IN(3)	70.00000	0.000000
T_AH_IN(4)	95.00000	0.000000
T_AH_OUT(1)	25.00000	0.000000
T_AH_OUT(2)	25.00000	0.000000
T_AH_OUT(3)	25.00000	0.000000
T_AH_OUT(4)	25.00000	0.000000
T_AC_IN(1)	25.00000	0.000000
T_AC_IN(2)	25.00000	0.000000
T_AC_IN(3)	80.00000	0.000000
T_AC_IN(4)	29.00000	0.000000
T_AC_OUT(1)	105.0000	0.000000
T_AC_OUT(2)	75.00000	0.000000
T_AC_OUT(3)	105.0000	0.000000
T_AC_OUT(4)	70.00000	0.000000
MCPH_A(1)	0.000000	0.000000
MCPH_A(2)	324.5568	0.000000
MCPH_A(3)	0.000000	0.000000
MCPH_A(4)	0.000000	0.000000
MCPC_A(1)	273.4164	0.000000
MCPC_A(2)	0.000000	0.000000
MCPC_A(3)	163.5679	0.000000
MCPC_A(4)	0.000000	0.000000
TP_A(1)	70.00000	0.000000
TP_A(2)	95.00000	0.000000
TP_A(3)	25.00000	0.000000
TP_A(4)	25.00000	0.000000
TP_A(5)	70.00000	0.000000
TP_A(6)	95.00000	0.000000
TP_A(7)	80.00000	0.000000
TP_A(8)	29.00000	0.000000
A(1)	14605.06	0.000000
A(2)	22718.98	0.000000
A(3)	0.000000	0.000000
A(4)	0.000000	0.000000
A(5)	14605.06	0.000000
A(6)	22718.98	0.000000
A(7)	17850.62	0.000000
A(8)	1298.227	0.000000
B(1)	12303.74	0.000000
B(2)	21592.67	0.000000
B(3)	0.000000	0.000000
B(4)	0.000000	0.000000
B(5)	12303.74	0.000000
B(6)	21592.67	0.000000
B(7)	15037.90	0.000000
B(8)	1093.666	0.000000
LAMSP(1, 1)	0.000000	0.000000
LAMSP(1, 2)	1.000000	0.000000
LAMSP(1, 3)	0.000000	0.000000
LAMSP(1, 4)	0.000000	0.000000
LAMSP(1, 5)	0.000000	0.000000
LAMSP(1, 6)	1.000000	0.000000
LAMSP(1, 7)	1.000000	0.000000
LAMSP(1, 8)	0.000000	0.000000
LAMSP(2, 1)	0.000000	0.000000
LAMSP(2, 2)	0.000000	0.000000
LAMSP(2, 3)	0.000000	0.000000

```
LAMSP( 2, 4)        0.000000        0.000000
LAMSP( 2, 5)        0.000000        0.000000
LAMSP( 2, 6)        0.000000        0.000000
LAMSP( 2, 7)        0.000000        486835.2
LAMSP( 2, 8)        0.000000        0.000000
LAMSP( 3, 1)        0.000000        0.000000
LAMSP( 3, 2)        1.000000        0.000000
LAMSP( 3, 3)        0.000000        0.000000
LAMSP( 3, 4)        0.000000        0.000000
LAMSP( 3, 5)        0.000000        0.000000
LAMSP( 3, 6)        1.000000        0.000000
LAMSP( 3, 7)        1.000000        0.000000
LAMSP( 3, 8)        0.000000        0.000000
LAMSP( 4, 1)        0.000000        0.000000
LAMSP( 4, 2)        0.000000        0.000000
LAMSP( 4, 3)        0.000000        0.000000
LAMSP( 4, 4)        0.000000        0.000000
LAMSP( 4, 5)        0.000000        0.000000
LAMSP( 4, 6)        0.000000        0.000000
LAMSP( 4, 7)        0.000000        0.000000
LAMSP( 4, 8)        0.000000        0.000000
LAMTP( 1, 1)        1.000000        0.000000
LAMTP( 1, 2)        1.000000        0.000000
LAMTP( 1, 3)        0.000000        0.000000
LAMTP( 1, 4)        0.000000        0.000000
LAMTP( 1, 5)        1.000000        0.000000
LAMTP( 1, 6)        1.000000        0.000000
LAMTP( 1, 7)        1.000000        0.000000
LAMTP( 1, 8)        1.000000        0.000000
LAMTP( 2, 1)        1.000000        0.000000
LAMTP( 2, 2)        1.000000        0.000000
LAMTP( 2, 3)        0.000000        0.000000
LAMTP( 2, 4)        0.000000        0.000000
LAMTP( 2, 5)        1.000000        0.000000
LAMTP( 2, 6)        1.000000        0.000000
LAMTP( 2, 7)        1.000000        1785062.
LAMTP( 2, 8)        1.000000        0.000000
LAMTP( 3, 1)        1.000000        0.000000
LAMTP( 3, 2)        1.000000        0.000000
LAMTP( 3, 3)        0.000000        0.000000
LAMTP( 3, 4)        0.000000        0.000000
LAMTP( 3, 5)        1.000000        0.000000
LAMTP( 3, 6)        1.000000        0.000000
LAMTP( 3, 7)        1.000000        0.000000
LAMTP( 3, 8)        1.000000        0.000000
LAMTP( 4, 1)        1.000000        0.000000
LAMTP( 4, 2)        1.000000        0.000000
LAMTP( 4, 3)        0.000000        0.000000
LAMTP( 4, 4)        0.000000        0.000000
LAMTP( 4, 5)        1.000000        0.000000
LAMTP( 4, 6)        1.000000        0.000000
LAMTP( 4, 7)        1.000000        0.000000
LAMTP( 4, 8)        1.000000        0.000000
  NSP( 1, 1)        1.000000        0.000000
  NSP( 1, 2)        1.000000        0.000000
  NSP( 1, 3)        0.000000        0.000000
  NSP( 1, 4)        0.000000        0.000000
  NSP( 1, 5)        1.000000        0.000000
  NSP( 1, 6)        1.000000        0.000000
  NSP( 1, 7)        1.000000       -1503782.
  NSP( 1, 8)        1.000000        0.000000
```

NSP(2, 1)	1.000000	0.000000
NSP(2, 2)	1.000000	0.000000
NSP(2, 3)	0.000000	0.000000
NSP(2, 4)	0.000000	0.000000
NSP(2, 5)	1.000000	0.000000
NSP(2, 6)	1.000000	0.000000
NSP(2, 7)	1.000000	-7.084077
NSP(2, 8)	1.000000	0.000000
NSP(3, 1)	0.000000	0.000000
NSP(3, 2)	1.000000	0.000000
NSP(3, 3)	0.000000	0.000000
NSP(3, 4)	0.000000	0.000000
NSP(3, 5)	0.000000	0.000000
NSP(3, 6)	1.000000	0.000000
NSP(3, 7)	0.000000	0.000000
NSP(3, 8)	0.000000	0.000000
NSP(4, 1)	1.000000	0.000000
NSP(4, 2)	1.000000	0.000000
NSP(4, 3)	0.000000	0.000000
NSP(4, 4)	0.000000	0.000000
NSP(4, 5)	1.000000	0.000000
NSP(4, 6)	1.000000	0.000000
NSP(4, 7)	1.000000	-6.568871
NSP(4, 8)	0.000000	0.000000
NTP(1, 1)	0.000000	0.000000
NTP(1, 2)	0.000000	0.000000
NTP(1, 3)	0.000000	0.000000
NTP(1, 4)	0.000000	0.000000
NTP(1, 5)	0.000000	0.000000
NTP(1, 6)	0.000000	0.000000
NTP(1, 7)	0.000000	-683537.4
NTP(1, 8)	0.000000	0.000000
NTP(2, 1)	0.000000	0.000000
NTP(2, 2)	1.000000	0.000000
NTP(2, 3)	0.000000	0.000000
NTP(2, 4)	0.000000	0.000000
NTP(2, 5)	0.000000	0.000000
NTP(2, 6)	1.000000	0.000000
NTP(2, 7)	1.000000	0.6440070
NTP(2, 8)	0.000000	0.000000
NTP(3, 1)	0.000000	0.000000
NTP(3, 2)	0.000000	0.000000
NTP(3, 3)	0.000000	0.000000
NTP(3, 4)	0.000000	0.000000
NTP(3, 5)	0.000000	0.000000
NTP(3, 6)	0.000000	0.000000
NTP(3, 7)	0.000000	-408919.8
NTP(3, 8)	0.000000	0.000000
NTP(4, 1)	0.000000	0.000000
NTP(4, 2)	1.000000	0.000000
NTP(4, 3)	0.000000	0.000000
NTP(4, 4)	0.000000	0.000000
NTP(4, 5)	0.000000	0.000000
NTP(4, 6)	1.000000	0.000000
NTP(4, 7)	1.000000	1.288014
NTP(4, 8)	0.000000	0.000000

APPENDIX F: HIRCN with heat of mixing mathematical model and solution for Case study 4 in Chapter 6

Appendix F1 – HIRCN with heat of mixing mathematical model for Case study 4

```
!Final coding after discretisation;

SETS:

SOURCES/1..5/      :F_R, C_R, VP_R, T_R,
                   FR_kg_phenol, FR_kgmol_phenol, FR_kg_water,
                   FR_kgmol_water, FR_x_phenol, FR_x_water,
                   FR_Cp, FR_Cp_water, FR_Cp_phenol;

SINKS/1..4/        :F_K, C_K, VP_K,  CK_in, TK_in,
                   FK_kg_phenol, FK_kgmol_phenol, FK_kg_water,
                   FK_kgmol_water, FK_x_phenol, FK_x_water,
                   FK_Cp, FK_Cp_water, FK_Cp_phenol, H_mixing, A12,
                   A21, molesink, Q, Fsk;

JUNCTIONS_A/1..4/  :C_A, F_A, VP_A, T_A, U,
                   FA_kg_phenol, FA_kgmol_phenol, FA_kg_water,
                   FA_kgmol_water, FA_x_phenol, FA_x_water,
                   FA_Cp, FA_Cp_water, FA_Cp_phenol, H_mixing_A,
                   A12_A, A21_A, molesink_A, Q_A;
                   !Junctions entering HEN_1;

JUNCTIONS_D/1..4/  :C_D, F_D, VP_D, T_D,
                   FD_kg_phenol, FD_kgmol_phenol, FD_kg_water,
                   FD_kgmol_water, FD_x_phenol, FD_x_water,
                   FD_Cp, FD_Cp_water, FD_Cp_phenol;
                   !Junctions exiting HEN_1;

STREAMS_RA(SOURCES, JUNCTIONS_A)          : F_RA;

STREAMS_DK(JUNCTIONS_D, SINKS)            : F_DK;

BYPASS_1(SOURCES, SINKS)                  : B_RK;

HEN_1/1..2/ : T_AH_IN, T_AH_OUT, T_AC_IN, T_AC_OUT, MCPH_A, MCPC_A;

PINCH_1/1..4/      : TP_A, A, B;

PINCH_BIN(HEN_1, PINCH_1): LAMSP, LAMTP, NSP, NTP;

ENDSETS

DATA:

!Concentration of sources;
C_R = 0.016 0.024 0.22 0 0.012;
!Constraints of source temperature;
T_R = 75 65 40 25 35;
```

```
!VP of source;
VP_R = 38 25 7 3 6;

ENDDATA

T_A(1) = T_R(1);
T_A(2) = T_R(2);
T_A(3) = T_R(3);
T_A(4) = T_R(4);

T_D(1) = 85;
T_D(2) = 40;
T_D(3) = 30;
T_D(4) = 55;

!Flowrate and concentration at JUNCTIONS_A is the same at
JUNCTIONS_D;
C_A(1) = C_D(1);
C_A(2) = C_D(2);
C_A(3) = C_D(3);
C_A(4) = C_D(4);

F_A(1) = F_D(1);
F_A(2) = F_D(2);
F_A(3) = F_D(3);
F_A(4) = F_D(4);

VP_A(1) = VP_D(1);
VP_A(2) = VP_D(2);
VP_A(3) = VP_D(3);
VP_A(4) = VP_D(4);

C_R(1) = C_A(1);
C_R(2) = C_A(2);
C_R(3) = C_A(3);
C_R(4) = C_A(4);

VP_R(1) = VP_A(1);
VP_R(2) = VP_A(2);
VP_R(3) = VP_A(3);
VP_R(4) = VP_A(4);

!Sink flowrate;
F_K(1) = 2718;
F_K(2) = 1993;
F_K(3) = 1127;

!Sink concentration;
CK_in(1) <= 0.013;
CK_in(2) <= 0.013;
CK_in(3) <= 0.1;

!Sink VP;
@BND(15, VP_K(1),35);
@BND(10, VP_K(2),25);
@BND(13, VP_K(3),40);

!Sink target temperatures;
@BND(70, TK_in(1), 85);
@BND(30, TK_in(2), 50);
@BND(25, TK_in(3), 65);
```

```
!Source Flowrate;
F_R(1) = 3661;
F_R(2) = 1766;
F_R(3) = 1485;

!molecular weight of phenol and water;
MW_phenol = 94.11;       !kg/kmol;
MW_water  = 18;          !kg/kmol;

!Objective function = minimise operation cost;
MIN = F_R(4)*Cost_AA + F_R(5)*Cost_SS + QH*Cost_HH + QC*Cost_CW +
F_K(4)*Cost_WW;

Cost_AA = 10.48; !$/kg;
Cost_SS = 7.04; !$/kg;
Cost_WW = 16.041663804; !$/yr;
Cost_CW = 20; !$/yr;
Cost_HH = 80;!$/yr;

!Mass Balance around sources;
@FOR (SOURCES(i):
      @SUM(JUNCTIONS_A(j):F_RA(i, j)) + @SUM(SINKS(l):B_RK(i, l)) =
      F_R(i));

!Mass Balance around junctions_A;
@FOR (JUNCTIONS_A(j):
      @SUM(SOURCES(i):F_RA(i, j)) = F_A(j));

!Composition Balance around junctions_A;
@FOR (JUNCTIONS_A(j):
      @SUM(SOURCES(i):F_RA(i, j)*C_R(i)) = F_A(j)*C_A(j));

!VP Balance around junctions_A;
@FOR (JUNCTIONS_A(j):
      @SUM(SOURCES(i):F_RA(i, j)*VP_R(i)) = F_A(j)*VP_A(j));

@FOR(JUNCTIONS_A(j):@SUM(STREAMS_RA(i,j): F_RA(i,j)*T_R(i)*FR_Cp(i))
= Q_A(j));

!Calculate T_A based on reuse/recycle stremas;
@FOR(JUNCTIONS_A(j): Q_A(j)/(F_A(j)*FA_Cp(j)) = T_A(j));

!Mass Balance around junctions_D;
@FOR (JUNCTIONS_D(k):
      @SUM(SINKS(l):F_DK(k, l)) = F_D(k));

!Mass Balance around sinks;
@FOR (SINKS(l):
      @SUM(JUNCTIONS_D(k):F_DK(k, l)) + @SUM(SOURCES(i):B_RK(i, l))
= F_K(l));

!Composition Balance around sinks;
@FOR (SINKS(l):
      @SUM(JUNCTIONS_D(k):F_DK(k, l)*C_D(k)) +
      @SUM(SOURCES(i):B_RK(i, l)*C_R(i)) = F_K(l)*CK_in(l));

!Sink VP load balance;
@FOR (SINKS(l):
      @SUM(JUNCTIONS_D(k):F_DK(k, l)*VP_D(k)) +
      @SUM(SOURCES(i):B_RK(i, l)*VP_R(i)) = F_K(l)*VP_K(l));
```

```
!Energy Balance around Sink;
!Calculate total energy received by each sink;
Q(1) = F_DK(1,1)*T_D(1)*FD_Cp(1) + F_DK(2,1)*T_D(2)*FD_Cp(2) +
F_DK(3,1)*T_D(3)*FD_Cp(3) + F_DK(4,1)*T_D(4)*FD_Cp(4) + H_mixing(1)
+ B_RK(1,1)*T_R(1)*FR_Cp(1) + B_RK(2,1)*T_R(2)*FR_Cp(2) +
B_RK(3,1)*T_R(3)*FR_Cp(3) + B_RK(4,1)*T_R(4)*FR_Cp(4) +
B_RK(5,1)*T_R(5)*FR_Cp(5);

Q(2) = F_DK(1,2)*T_D(1)*FD_Cp(1) + F_DK(2,2)*T_D(2)*FD_Cp(2) +
F_DK(3,2)*T_D(3)*FD_Cp(3) + F_DK(4,2)*T_D(4)*FD_Cp(4) + H_mixing(2)
+ B_RK(1,2)*T_R(1)*FR_Cp(1) + B_RK(2,2)*T_R(2)*FR_Cp(2) +
B_RK(3,2)*T_R(3)*FR_Cp(3) + B_RK(4,2)*T_R(4)*FR_Cp(4) +
B_RK(5,2)*T_R(5)*FR_Cp(5) ;

Q(3) = F_DK(1,3)*T_D(1)*FD_Cp(1) + F_DK(2,3)*T_D(2)*FD_Cp(2) +
F_DK(3,3)*T_D(3)*FD_Cp(3) + F_DK(4,3)*T_D(4)*FD_Cp(4) + H_mixing(3)
+ B_RK(1,3)*T_R(1)*FR_Cp(1) + B_RK(2,3)*T_R(2)*FR_Cp(2) +
B_RK(3,3)*T_R(3)*FR_Cp(3) + B_RK(4,3)*T_R(4)*FR_Cp(4) +
B_RK(5,3)*T_R(5)*FR_Cp(5);

Q(4) = F_DK(1,4)*T_D(1)*FD_Cp(1) + F_DK(2,4)*T_D(2)*FD_Cp(2) +
F_DK(3,4)*T_D(3)*FD_Cp(3) + F_DK(4,4)*T_D(4)*FD_Cp(4) + H_mixing(3)
+ B_RK(1,4)*T_R(1)*FR_Cp(1) + B_RK(2,4)*T_R(2)*FR_Cp(2) +
B_RK(3,4)*T_R(3)*FR_Cp(3) + B_RK(4,4)*T_R(4)*FR_Cp(4) +
B_RK(5,4)*T_R(5)*FR_Cp(5);

!no fresh bypass to waste;
B_RK(4,4) = 0;
B_RK(5,4) = 0;

!Calculate Tsink based on reuse/recycle stremas;
@FOR(SINKS(l): Q(l)/(F_K(l)*FK_Cp(l)) = TK_in(l));

!Cp calculation for process sources;
@FOR(SOURCES(i):FR_kg_phenol(i) = 100 * C_R(i));

@FOR(SOURCES(i):FR_kg_water(i)  = 100 - FR_kg_phenol(i));

@FOR(SOURCES(i):FR_kgmol_phenol(i) = FR_kg_phenol(i)/ MW_phenol);

@FOR(SOURCES(i):FR_kgmol_water(i)  = FR_kg_water(i) / MW_water);

@FOR(SOURCES(i):FR_x_phenol(i) = FR_kgmol_phenol(i) /
(FR_kgmol_water(i) + FR_kgmol_phenol(i)));

@FOR(SOURCES(i):FR_x_water(i)  = FR_kgmol_water(i)  /
(FR_kgmol_water(i) + FR_kgmol_phenol(i)));

@FOR(SOURCES(i):FR_x_phenol(i) <=1);

@FOR(SOURCES(i):FR_x_water(i)  <=1);

@FOR(SOURCES(i):FR_Cp(i) = FR_x_water(i)*FR_Cp_water(i) +
FR_x_phenol(i)*FR_Cp_phenol(i));    !J/g.K;

@FOR(SOURCES(i):FR_Cp_water(i)  = 1.3724 + 0.0083 * T_R(i));
                  !J/g.K;

@FOR(SOURCES(i):FR_Cp_phenol(i) = 0.4685 + 0.0044 * T_R(i));
                  !J/g.K;
```

```
!Cp calculation for junction A;
@FOR(JUNCTIONS_A(j):FA_kg_phenol(j) = 100 * C_A(j));

@FOR(JUNCTIONS_A(j):FA_kg_water(j)  = 100 - FA_kg_phenol(j));

@FOR(JUNCTIONS_A(j):FA_kgmol_phenol(j) = FA_kg_phenol(j)/
MW_phenol);
@FOR(JUNCTIONS_A(j):FA_kgmol_water(j)  = FA_kg_water(j) / MW_water);

@FOR(JUNCTIONS_A(j):FA_x_phenol(j) = FA_kgmol_phenol(j) /
(FA_kgmol_water(j) + FA_kgmol_phenol(j)));

@FOR(JUNCTIONS_A(j):FA_x_water(j)  = FA_kgmol_water(j)  /
(FA_kgmol_water(j) + FA_kgmol_phenol(j)));

@FOR(JUNCTIONS_A(j):FA_x_phenol(j) <=1);

@FOR(JUNCTIONS_A(j):FA_x_water(j)  <=1);

@FOR(JUNCTIONS_A(j):FA_Cp(j) = FA_x_water(j)*FA_Cp_water(j) +
FA_x_phenol(j)*FA_Cp_phenol(j));    !J/g.K;

@FOR(JUNCTIONS_A(j):FA_Cp_water(j)  = 1.3724 + 0.0083 * T_A(j));
                  !J/g.K;

@FOR(JUNCTIONS_A(j):FA_Cp_phenol(j) = 0.4685 + 0.0044 * T_A(j));

FD_Cp(1) = FA_Cp(1);
FD_Cp(2) = FA_Cp(2);
FD_Cp(3) = FA_Cp(3);
FD_Cp(4) = FA_Cp(4);

!Cp calculation for process sinks;
@FOR(SINKS(l):FK_kg_phenol(l) = 100*CK_in(l));

@FOR(SINKS(l):FK_kg_water(l)  = 100 - FK_kg_phenol(l));

@FOR(SINKS(l):FK_kgmol_phenol(l) = FK_kg_phenol(l)/ MW_phenol);

@FOR(SINKS(l):FK_kgmol_water(l)  = FK_kg_water(l) / MW_water);

@FOR(SINKS(l):FK_x_phenol(l) = FK_kgmol_phenol(l) /
(FK_kgmol_water(l) + FK_kgmol_phenol(l)));

@FOR(SINKS(l):FK_x_water(l)  = FK_kgmol_water(l)  /
(FK_kgmol_water(l) + FK_kgmol_phenol(l)));

@FOR(SINKS(l):FK_x_phenol(l) <=1);

@FOR(SINKS(l):FK_x_water(l)  <=1);

@FOR(SINKS(l):FK_Cp(l) = FK_x_water(l)*FK_Cp_water(l) +
FK_x_phenol(l)*FK_Cp_phenol(l));    !J/g.K;

@FOR(SINKS(l):FK_Cp_water(l)  = 1.3724 + 0.0083 * TK_in(l));
                  !J/g.K;

@FOR(SINKS(l):FK_Cp_phenol(l) = 0.4685 + 0.0044 * TK_in(l));
!Heat of mixing calculation at Junction A;
@FOR(JUNCTIONS_A(j):H_mixing_A(j) =       - 8.314 *
FA_x_phenol(j)*FA_x_water(j)*molesink_A(j)*
```

```
((A12_A(j)*(-2229.9297))/(FA_x_phenol(j) + FA_x_water(j) *A12_A(j))
+ (A21_A(j)*( 1046.1246))/(FA_x_water(j)  +
FA_x_phenol(j)*A21_A(j))));

@FOR(JUNCTIONS_A(j):molesink_A(j) = (F_A(j)*C_A(j))/MW_phenol +
(F_A(j)*(1-C_A(j)))/MW_water);

@FOR(JUNCTIONS_A(j):A12_A(j) = @EXP( 2.4395 - 2229.9297 / (T_A(j) +
273.15)));

@FOR(JUNCTIONS_A(j):A21_A(j) = @EXP(-3.2239 + 1046.1246 / (T_A(j) +
273.15)));

@FOR(JUNCTIONS_A(j):@FREE(A); @FREE(B); @FREE(H_mixing_A));

!Heat of mixing calculation at sink;
@FOR(SINKS(l):H_mixing(l) =   - 8.314 *
FK_x_phenol(l)*FK_x_water(l)*molesink(l)*
((A12(l)*(-2229.9297))/(FK_x_phenol(l) + FK_x_water(l) *A12(l)) +
(A21(l)*( 1046.1246))/(FK_x_water(l)  + FK_x_phenol(l)*A21(l))));

@FOR(SINKS(l):molesink(l) = (F_K(l)*CK_in(l))/MW_phenol +
(F_K(l)*(1-CK_in(l)))/MW_water);

@FOR(SINKS(l):A12(l) = @EXP( 2.4395 - 2229.9297 / (TK_in(l) +
273.15)));

@FOR(SINKS(l):A21(l) = @EXP(-3.2239 + 1046.1246 / (TK_in(l) +
273.15)));

@FOR(SINKS(l):@FREE(A); @FREE(B); @FREE(H_mixing));

!Set the maximum of F_A;
@FOR(JUNCTIONS_A(j): F_A(j) <= 2718*U(j));

!Only have 4 junctions;
@SUM(JUNCTIONS_A(j): U(j)) = 2;

!U(j) is binary variable;
@FOR(JUNCTIONS_A(j): @BIN (U(j)));

!Minimum temperature difference;
DT = 10;

!Identifying (shifted temperatures) hot and cold streams;
 T_AH_IN(1)*2  = T_A(3)*2 - DT;
T_AH_OUT(1)*2  = T_D(3)*2 - DT;
 T_AH_IN(2)*2  = T_A(2)*2 - DT;
T_AH_OUT(2)*2  = T_D(2)*2 - DT;

 T_AC_IN(1)*2  = T_A(1)*2 + DT;
T_AC_OUT(1)*2  = T_D(1)*2 + DT;
 T_AC_IN(2)*2  = T_A(4)*2 + DT;
T_AC_OUT(2)*2  = T_D(4)*2 + DT;

!MCP values;
MCPH_A(1) = FA_Cp(3)*F_A(3);
MCPH_A(2) = FA_Cp(2)*F_A(2);
MCPC_A(1) = FA_Cp(1)*F_A(1);
MCPC_A(2) = FA_Cp(4)*F_A(4);
```

```
!Assigning pinch temperatures = supply temperatures;
TP_A(1) = T_AH_IN(1);
TP_A(2) = T_AH_IN(2);
TP_A(3) = T_AC_IN(1);
TP_A(4) = T_AC_IN(2);

!Identifying pinch location (BIN=1 below pinch, BIN=0, above pinch);
@FOR (PINCH_BIN(m, n):
      (0-TP_A(n))*LAMSP(m, n) < T_AH_IN(m)-TP_A(n);
      (10e6-TP_A(n))*(1-LAMSP(m, n)) >= T_AH_IN(m)-TP_A(n);

      (0-TP_A(n))*LAMTP(m, n) < T_AH_OUT(m)-TP_A(n);
      (10e6-TP_A(n))*(1-LAMTP(m, n)) >= T_AH_OUT(m)-TP_A(n);

      (0-TP_A(n))*NSP(m, n) < T_AC_IN(m)-TP_A(n);
      (10e6-TP_A(n))*(1-NSP(m, n)) >= T_AC_IN(m)-TP_A(n);

      (0-TP_A(n))*NTP(m, n) < T_AC_OUT(m)-TP_A(n);
      (10e6-TP_A(n))*(1-NTP(m, n)) >= T_AC_OUT(m)-TP_A(n));

@FOR (PINCH_1(n):
      @SUM(HEN_1(m):MCPH_A(m)*(LAMTP(m, n)*(TP_A(n)-T_AH_OUT(m))-
      LAMSP(m, n)*(TP_A(n)-T_AH_IN(m)))) = A(n);

      @SUM(HEN_1(o):MCPC_A(o)*(NSP(o, n)*(TP_A(n)-T_AC_IN(o))-NTP(o,
      n)*(TP_A(n)-T_AC_OUT(o)))) = B(n);

      A(n) - B(n) <= QC);

!Overall energy balance;
@SUM(HEN_1(m):MCPH_A(m)*(T_AH_IN(m)-T_AH_OUT(m))) -
@SUM(HEN_1(m):MCPC_A(m)*(T_AC_OUT(m)-T_AC_IN(m))) + QH - QC = 0;

!Defining binary integers;
@FOR (PINCH_BIN(m, n):@BIN(LAMTP(m,n)); @BIN(LAMSP(m,n));
@BIN(NTP(m,n)); @BIN(NSP(m,n)));

!each source only supply to one junction;
F_RA(1,3) = 0;
F_RA(1,4) = 0;
F_RA(2,1) = 0;
F_RA(2,3) = 0;
F_RA(2,4) = 0;
F_RA(3,1) = 0;
F_RA(3,2) = 0;
F_RA(3,4) = 0;
F_RA(4,1) = 0;
F_RA(4,2) = 0;
F_RA(4,3) = 0;

end
```

Appendix F2 – HIRCN with heat of mixing solution for Case study 4

```
Global optimal solution found.
  Objective value:                              49958.91
  Objective bound:                              49958.91
  Infeasibilities:                              0.000000
  Extended solver steps:                               1
  Total solver iterations:                      12339606

  Model Class:                                     MINLP

  Total variables:                    235
  Nonlinear variables:                108
  Integer variables:                   36

  Total constraints:                  224
  Nonlinear constraints:               51

  Total nonzeros:                     604
  Nonlinear nonzeros:                 157


                       Variable           Value
                      MW_PHENOL        94.11000
                       MW_WATER        18.00000
                        COST_AA        10.48000
                        COST_SS        7.040000
                             QH        0.000000
                        COST_HH        80.00000
                             QC        0.000000
                        COST_CW        20.00000
                        COST_WW        16.04166
                             DT        10.00000
                        F_R( 1)        3661.000
                        F_R( 2)        1766.000
                        F_R( 3)        1485.000
                        F_R( 4)        1234.092
                        F_R( 5)        0.000000
                        C_R( 1)       0.1600000E-01
                        C_R( 2)       0.2400000E-01
                        C_R( 3)       0.2200000
                        C_R( 4)        0.000000
                        C_R( 5)       0.1200000E-01
                       VP_R( 1)        38.00000
                       VP_R( 2)        25.00000
                       VP_R( 3)        7.000000
                       VP_R( 4)        3.000000
                       VP_R( 5)        6.000000
                        T_R( 1)        75.00000
                        T_R( 2)        65.00000
                        T_R( 3)        40.00000
                        T_R( 4)        25.00000
                        T_R( 5)        35.00000
               FR_KG_PHENOL( 1)        1.600000
               FR_KG_PHENOL( 2)        2.400000
               FR_KG_PHENOL( 3)        22.00000
               FR_KG_PHENOL( 4)        0.000000
               FR_KG_PHENOL( 5)        1.200000
            FR_KGMOL_PHENOL( 1)       0.1700138E-01
            FR_KGMOL_PHENOL( 2)       0.2550207E-01
```

```
FR_KGMOL_PHENOL( 3)        0.2337690
FR_KGMOL_PHENOL( 4)         0.000000
FR_KGMOL_PHENOL( 5)        0.1275104E-01
    FR_KG_WATER( 1)         98.40000
    FR_KG_WATER( 2)         97.60000
    FR_KG_WATER( 3)         78.00000
    FR_KG_WATER( 4)         100.0000
    FR_KG_WATER( 5)         98.80000
 FR_KGMOL_WATER( 1)         5.466667
 FR_KGMOL_WATER( 2)         5.422222
 FR_KGMOL_WATER( 3)         4.333333
 FR_KGMOL_WATER( 4)         5.555556
 FR_KGMOL_WATER( 5)         5.488889
    FR_X_PHENOL( 1)        0.3100367E-02
    FR_X_PHENOL( 2)        0.4681234E-02
    FR_X_PHENOL( 3)        0.5118541E-01
    FR_X_PHENOL( 4)         0.000000
    FR_X_PHENOL( 5)        0.2317679E-02
     FR_X_WATER( 1)        0.9968996
     FR_X_WATER( 2)        0.9953188
     FR_X_WATER( 3)        0.9488146
     FR_X_WATER( 4)         1.000000
     FR_X_WATER( 5)        0.9976823
          FR_CP( 1)         1.991191
           R_CP( 2)         1.906482
          FR_CP( 3)         1.650149
          FR_CP( 4)         1.579900
          FR_CP( 5)         1.660489
    FR_CP_WATER( 1)         1.994900
    FR_CP_WATER( 2)         1.911900
    FR_CP_WATER( 3)         1.704400
    FR_CP_WATER( 4)         1.579900
    FR_CP_WATER( 5)         1.662900
   FR_CP_PHENOL( 1)        0.7985000
   FR_CP_PHENOL( 2)        0.7545000
   FR_CP_PHENOL( 3)        0.6445000
   FR_CP_PHENOL( 4)        0.5785000
   FR_CP_PHENOL( 5)        0.6225000
           F_K( 1)          2718.000
           F_K( 2)          1993.000
           F_K( 3)          1127.000
           F_K( 4)          2308.092
           C_K( 1)          0.000000
           C_K( 2)          0.000000
           C_K( 3)          0.000000
           C_K( 4)          0.000000
          VP_K( 1)          31.43750
          VP_K( 2)          20.70116
          VP_K( 3)          24.49285
          VP_K( 4)          18.65493
         CK_IN( 1)         0.1300000E-01
         CK_IN( 2)         0.1300000E-01
         CK_IN( 3)         0.3305692E-01
         CK_IN( 4)         0.1426121
         TK_IN( 1)          70.92256
         TK_IN( 2)          50.00000
         TK_IN( 3)          65.00000
         TK_IN( 4)          54.85312
   FK_KG_PHENOL( 1)         1.300000
   FK_KG_PHENOL( 2)         1.300000
   FK_KG_PHENOL( 3)         3.305692
```

```
   FK_KG_PHENOL( 4)         14.26121
FK_KGMOL_PHENOL( 1)        0.1381362E-01
FK_KGMOL_PHENOL( 2)        0.1381362E-01
FK_KGMOL_PHENOL( 3)        0.3512584E-01
FK_KGMOL_PHENOL( 4)        0.1515377
    FK_KG_WATER( 1)         98.70000
    FK_KG_WATER( 2)         98.70000
    FK_KG_WATER( 3)         96.69431
    FK_KG_WATER( 4)         85.73879
 FK_KGMOL_WATER( 1)         5.483333
 FK_KGMOL_WATER( 2)         5.483333
 FK_KGMOL_WATER( 3)         5.371906
 FK_KGMOL_WATER( 4)         4.763266
    FK_X_PHENOL( 1)        0.2512871E-02
    FK_X_PHENOL( 2)        0.2512871E-02
    FK_X_PHENOL( 3)        0.6496325E-02
    FK_X_PHENOL( 4)        0.3083291E-01
     FK_X_WATER( 1)        0.9974871
     FK_X_WATER( 2)        0.9974871
     FK_X_WATER( 3)        0.9935037
     FK_X_WATER( 4)        0.9691671
          FK_CP( 1)         1.958091
          FK_CP( 2)         1.784639
          FK_CP( 3)         1.904381
          FK_CP( 4)         1.793215
    FK_CP_WATER( 1)         1.961057
    FK_CP_WATER( 2)         1.787400
    FK_CP_WATER( 3)         1.911900
    FK_CP_WATER( 4)         1.827681
   FK_CP_PHENOL( 1)        0.7805593
   FK_CP_PHENOL( 2)        0.6885000
   FK_CP_PHENOL( 3)        0.7545000
   FK_CP_PHENOL( 4)        0.7098537
       H_MIXING( 1)         3375.542
       H_MIXING( 2)         1769.597
       H_MIXING( 3)         2174.553
       H_MIXING( 4)        -9916.668
            A12( 1)        0.1757133E-01
            A12( 2)        0.1154962E-01
            A12( 3)        0.1568581E-01
            A12( 4)        0.1279115E-01
            A21( 1)        0.8323673
            A21( 2)         1.013462
            A21( 3)        0.8778937
            A21( 4)        0.9660631
       MOLESINK( 1)         149.4125
       MOLESINK( 2)         109.5581
       MOLESINK( 3)         60.93725
       MOLESINK( 4)         113.4382
              Q( 1)         377456.3
              Q( 2)         177839.2
              Q( 3)         139505.4
              Q( 4)         227031.8
            FSK( 1)         0.000000
            FSK( 2)         0.000000
            FSK( 3)         0.000000
            FSK( 4)         0.000000
            C_A( 1)        0.1600000E-01
            C_A( 2)        0.2400000E-01
            C_A( 3)        0.2200000
            C_A( 4)         0.000000
```

```
            F_A( 1)        0.000000
            F_A( 2)        506.7910
            F_A( 3)        0.000000
            F_A( 4)        509.6250
           VP_A( 1)        38.00000
           VP_A( 2)        25.00000
           VP_A( 3)        7.000000
           VP_A( 4)        3.000000
            T_A( 1)        75.00000
            T_A( 2)        65.00000
            T_A( 3)        40.00000
            T_A( 4)        25.00000
              U( 1)        0.000000
              U( 2)        1.000000
              U( 3)        0.000000
              U( 4)        1.000000
   FA_KG_PHENOL( 1)        1.600000
   FA_KG_PHENOL( 2)        2.400000
   FA_KG_PHENOL( 3)        22.00000
   FA_KG_PHENOL( 4)        0.000000
FA_KGMOL_PHENOL( 1)       0.1700138E-01
FA_KGMOL_PHENOL( 2)       0.2550207E-01
FA_KGMOL_PHENOL( 3)       0.2337690
FA_KGMOL_PHENOL( 4)        0.000000
    FA_KG_WATER( 1)        98.40000
    FA_KG_WATER( 2)        97.60000
    FA_KG_WATER( 3)        78.00000
    FA_KG_WATER( 4)        100.0000
 FA_KGMOL_WATER( 1)        5.466667
 FA_KGMOL_WATER( 2)        5.422222
 FA_KGMOL_WATER( 3)        4.333333
 FA_KGMOL_WATER( 4)        5.555556
    FA_X_PHENOL( 1)       0.3100367E-02
    FA_X_PHENOL( 2)       0.4681234E-02
    FA_X_PHENOL( 3)       0.5118541E-01
    FA_X_PHENOL( 4)        0.000000
     FA_X_WATER( 1)       0.9968996
     FA_X_WATER( 2)       0.9953188
     FA_X_WATER( 3)       0.9488146
     FA_X_WATER( 4)        1.000000
          FA_CP( 1)        1.991191
          FA_CP( 2)        1.906482
          FA_CP( 3)        1.650149
          FA_CP( 4)        1.579900
    FA_CP_WATER( 1)        1.994900
    FA_CP_WATER( 2)        1.911900
    FA_CP_WATER( 3)        1.704400
    FA_CP_WATER( 4)        1.579900
   FA_CP_PHENOL( 1)       0.7985000
   FA_CP_PHENOL( 2)       0.7545000
   FA_CP_PHENOL( 3)       0.6445000
   FA_CP_PHENOL( 4)       0.5785000
     H_MIXING_A( 1)        0.000000
     H_MIXING_A( 2)        0.000000
     H_MIXING_A( 3)        0.000000
     H_MIXING_A( 4)        0.000000
          A12_A( 1)        0.000000
          A12_A( 2)        0.000000
          A12_A( 3)        0.000000
          A12_A( 4)        0.000000
          A21_A( 1)        0.000000
```

```
          A21_A( 2)        0.000000
          A21_A( 3)        0.000000
          A21_A( 4)        0.000000
     MOLESINK_A( 1)        0.000000
     MOLESINK_A( 2)        0.000000
     MOLESINK_A( 3)        0.000000
     MOLESINK_A( 4)        0.000000
            Q_A( 1)       0.2502724E-08
            Q_A( 2)        62802.21
            Q_A( 3)        0.000000
            Q_A( 4)        20128.91
            C_D( 1)       0.1600000E-01
            C_D( 2)       0.2400000E-01
            C_D( 3)       0.2200000
            C_D( 4)        0.000000
            F_D( 1)        0.000000
            F_D( 2)        506.7910
            F_D( 3)        0.000000
            F_D( 4)        509.6250
           VP_D( 1)        38.00000
           VP_D( 2)        25.00000
           VP_D( 3)        7.000000
           VP_D( 4)        3.000000
            T_D( 1)        85.00000
            T_D( 2)        40.00000
            T_D( 3)        30.00000
            T_D( 4)        55.00000
   FD_KG_PHENOL( 1)        0.000000
   FD_KG_PHENOL( 2)        0.000000
   FD_KG_PHENOL( 3)        0.000000
   FD_KG_PHENOL( 4)        0.000000
FD_KGMOL_PHENOL( 1)        0.000000
FD_KGMOL_PHENOL( 2)        0.000000
FD_KGMOL_PHENOL( 3)        0.000000
FD_KGMOL_PHENOL( 4)        0.000000
    FD_KG_WATER( 1)        0.000000
    FD_KG_WATER( 2)        0.000000
    FD_KG_WATER( 3)        0.000000
    FD_KG_WATER( 4)        0.000000
 FD_KGMOL_WATER( 1)        0.000000
 FD_KGMOL_WATER( 2)        0.000000
 FD_KGMOL_WATER( 3)        0.000000
 FD_KGMOL_WATER( 4)        0.000000
    FD_X_PHENOL( 1)        0.000000
    FD_X_PHENOL( 2)        0.000000
    FD_X_PHENOL( 3)        0.000000
    FD_X_PHENOL( 4)        0.000000
     FD_X_WATER( 1)        0.000000
     FD_X_WATER( 2)        0.000000
     FD_X_WATER( 3)        0.000000
     FD_X_WATER( 4)        0.000000
          FD_CP( 1)        1.991191
          FD_CP( 2)        1.906482
          FD_CP( 3)        1.650149
          FD_CP( 4)        1.579900
    FD_CP_WATER( 1)        0.000000
    FD_CP_WATER( 2)        0.000000
    FD_CP_WATER( 3)        0.000000
    FD_CP_WATER( 4)        0.000000
   FD_CP_PHENOL( 1)        0.000000
   FD_CP_PHENOL( 2)        0.000000
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```
FD_CP_PHENOL( 3)        0.000000
FD_CP_PHENOL( 4)        0.000000
     F_RA( 1, 1)        0.000000
     F_RA( 1, 2)        0.000000
     F_RA( 1, 3)        0.000000
     F_RA( 1, 4)        0.000000
     F_RA( 2, 1)        0.000000
     F_RA( 2, 2)        506.7910
     F_RA( 2, 3)        0.000000
     F_RA( 2, 4)        0.000000
     F_RA( 3, 1)        0.000000
     F_RA( 3, 2)        0.000000
     F_RA( 3, 3)        0.000000
     F_RA( 3, 4)        0.000000
     F_RA( 4, 1)        0.000000
     F_RA( 4, 2)        0.000000
     F_RA( 4, 3)        0.000000
     F_RA( 4, 4)        509.6250
     F_RA( 5, 1)        0.000000
     F_RA( 5, 2)        0.000000
     F_RA( 5, 3)        0.000000
     F_RA( 5, 4)        0.000000
     F_DK( 1, 1)        0.000000
     F_DK( 1, 2)        0.000000
     F_DK( 1, 3)        0.000000
     F_DK( 1, 4)        0.000000
     F_DK( 2, 1)        0.000000
     F_DK( 2, 2)        506.7910
     F_DK( 2, 3)        0.000000
     F_DK( 2, 4)        0.000000
     F_DK( 3, 1)        0.000000
     F_DK( 3, 2)        0.000000
     F_DK( 3, 3)        0.000000
     F_DK( 3, 4)        0.000000
     F_DK( 4, 1)        509.6250
     F_DK( 4, 2)        0.000000
     F_DK( 4, 3)        0.000000
     F_DK( 4, 4)        0.000000
     B_RK( 1, 1)        2208.375
     B_RK( 1, 2)        566.9754
     B_RK( 1, 3)        29.82688
     B_RK( 1, 4)        855.8227
     B_RK( 2, 1)        0.000000
     B_RK( 2, 2)        194.7671
     B_RK( 2, 3)        1043.878
     B_RK( 2, 4)        20.56358
     B_RK( 3, 1)        0.000000
     B_RK( 3, 2)        0.000000
     B_RK( 3, 3)        53.29474
     B_RK( 3, 4)        1431.705
     B_RK( 4, 1)        0.000000
     B_RK( 4, 2)        724.4665
     B_RK( 4, 3)        0.000000
     B_RK( 4, 4)        0.000000
     B_RK( 5, 1)        0.000000
     B_RK( 5, 2)        0.000000
     B_RK( 5, 3)        0.000000
     B_RK( 5, 4)        0.000000
     T_AH_IN( 1)        35.00000
     T_AH_IN( 2)        60.00000
    T_AH_OUT( 1)        25.00000
```

```
T_AH_OUT( 2)          35.00000
 T_AC_IN( 1)          80.00000
 T_AC_IN( 2)          30.00000
T_AC_OUT( 1)          90.00000
T_AC_OUT( 2)          60.00000
  MCPH_A( 1)          0.000000
  MCPH_A( 2)          966.1878
  MCPC_A( 1)          0.000000
  MCPC_A( 2)          805.1565
    TP_A( 1)          35.00000
    TP_A( 2)          60.00000
    TP_A( 3)          80.00000
    TP_A( 4)          30.00000
       A( 1)          0.000000
       A( 2)          24154.70
       A( 3)          24154.70
       A( 4)          0.000000
       B( 1)          4025.783
       B( 2)          24154.70
       B( 3)          24154.70
       B( 4)          0.000000
LAMSP( 1, 1)          0.000000
LAMSP( 1, 2)          1.000000
LAMSP( 1, 3)          1.000000
LAMSP( 1, 4)          0.000000
LAMSP( 2, 1)          0.000000
LAMSP( 2, 2)          0.000000
LAMSP( 2, 3)          1.000000
LAMSP( 2, 4)          0.000000
LAMTP( 1, 1)          1.000000
LAMTP( 1, 2)          1.000000
LAMTP( 1, 3)          1.000000
LAMTP( 1, 4)          1.000000
LAMTP( 2, 1)          0.000000
LAMTP( 2, 2)          1.000000
LAMTP( 2, 3)          1.000000
LAMTP( 2, 4)          0.000000
  NSP( 1, 1)          0.000000
  NSP( 1, 2)          0.000000
  NSP( 1, 3)          0.000000
  NSP( 1, 4)          0.000000
  NSP( 2, 1)          1.000000
  NSP( 2, 2)          1.000000
  NSP( 2, 3)          1.000000
  NSP( 2, 4)          0.000000
  NTP( 1, 1)          0.000000
  NTP( 1, 2)          0.000000
  NTP( 1, 3)          0.000000
  NTP( 1, 4)          0.000000
  NTP( 2, 1)          0.000000
  NTP( 2, 2)          0.000000
  NTP( 2, 3)          1.000000
  NTP( 2, 4)          0.000000
```